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This document presents Urban Airshed Modeling results for St. Louis and Philadelphia. Two sets of meteorological inputs, representing rich and sparse observed data fields, were developed for each city. Comparison simulations based on the different input approaches are presented.

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1 INTRODUCTION

The job of reducing ozone concentrations to levels below the National Ambient Air Quality Standard (NAAQS) has proven to be far more difficult than was thought when the Clean Air Act was passed and amended. The level of ozone precursor emissions remains too high; either emission reductions have been too small or have been required of the wrong sources, or both.

A plethora of technical explanations has been offered for failure to attain the ozone standard. These include perceived weaknesses in the attainment planning process (Federal Registrar, Vol. 52, No. 226, November 24, 1987; OTA 1988a,b,c), incomplete understanding or recognition of the anthropogenic and natural factors that cause elevated tropospheric ozone levels (Science, 1988), the failure to consider the effects of natural emissions (Chameides et al., 1988; Morris et al., 1989), use of a simplistic modeling approach (OTA, 1988a; Seinfeld, 1988a; Burton, 1988), and failure to reduce the amount of emissions intended, either through overestimates of the effectiveness of control technology or failure to account for certain categories of emission sources. The EPA, after lengthy consideration, has proposed a comprehensive policy that includes major changes in the planning process for reducing ozone concentrations (Federal Registrar, Vol. 52, No. 226, November 24, 1987). These changes include improvements in modeling practices and requirements for improving the data to support improved modeling practices. The EPA is now evaluating public comments on the proposed policy.

USE OF THE URBAN AIRSHED MODEL

The EPA has recommended the Urban Airshed Model (UAM) as the preferred approach for estimating emission controls needed to attain the ozone NAAQS. However, in the past there has been a reluctance to use the UAM because of the perception that it requires using data from costly intensive measurement studies and requires extensive computational resources. Most of the cost of applying the UAM is attributed to the practice of conducting an extensive evaluation of UAM performance, which usually entails many diagnostic simulations. This evaluation enables us to understand why the UAM performs as it does for a particular application and, if deemed necessary, to take actions to improve model performance. Historically, it has been expected that the UAM will calculate hourly ozone concentrations to within approximately 15 to 20 percent of the observed peak value (Seinfeld, 1988a; Burton, 1988). More recent applications of the UAM to the Los Angeles basin have used routinely available meteorological data and predicted observed ozone levels with a high degree of skill (Seinfeld, 1988a; Burton, 1988; Hogo, Mahoney, and Yocke 1988). A recent application of the UAM to the New York metropolitan area used simple inputs, i.e., constant wind fields and mixing depths (Rao 1987).

This simplified use of the UAM, relying on routinely available data and reducing the requirement for strict evaluations of model performance, offers air quality managers a practical air quality assessment tool for identifying emission control strategies that demonstrate attainment of the ozone NAAQS. This simplified approach is called Practice-for-Low-Cost-Airshed-Application-for-Nonattainment-Regions (PLANR). The PLANR use of the UAM requires almost the same quantity and quality of inputs as EKMA, and the overall application cost is substantially reduced. The possible exception is the emissions inventory, which in PLANR applications should contain the same spatially (horizontally and vertically) and temporally varying emissions used in standard UAM applications (such detail is necessary to account for the differing reactivities of VOC emissions). However, local agencies generally have emissions inventories at hand; in addition, UAM input inventories can be readily estimated from existing national emissions inventories (e.g., the National Acid Precipitation Program 1980 and 1985 inventories). Knowledge of current emission rates is needed to estimate the emission controls required to achieve attainment of the ozone NAAQS.

The PLANR use of the UAM may not be appropriate for all nonattainment regions. When attainment is expected to be imminent, improved methods for using EKMA may be adequate. In other, more complex situations, such as the Los Angeles basin, the Houston region, and the New York Metropolitan area among others, the complexity of meteorological conditions and the emissions distribution and the severity of the ozone attainment problem probably require a more detailed application of the UAM. The application of UAM to these more complex situations, called Practice-of-Airshed-Application-in-Complex-Regions (PACR), would involve more extensive model performance requirements and hence more diagnostic simulations, and a resultant increase in costs. However, even for a complex nonattainment region, the PLANR approach would probably be more comprehensive and reliable than EKMA for estimating the controls needed to achieve ozone attainment.

THE "FIVE CITIES" UAM STUDY

The EPA has funded a study of the PLANR approach in five urban areas in the U.S. (New York, St. Louis, Atlanta, Philadelphia, and Dallas-Ft. Worth). The main objectives of this "Five Cities" study are to:

(1) Demonstrate the usefulness of PLANR for air quality planning;

(2) Determine the effects of alternative fuels and alternative Reid vapor pressure values for fuels on urban ozone concentrations;

(3) Demonstrate the use of PLANR to evaluate SIP control strategies and compare results with those obtained with EKMA; and

(4) Transfer the UAM model, modeling data bases, and applications technology to the states for use in future SIPs.

In addition, the study includes two city-specific analyses:

(1) For the St. Louis and Philadelphia areas, comparison of the PLANR use of the UAM (i.e., using only routinely available data) with applications of the UAM that use an extensive data base; and

(2) The effects of biogenic emissions on anthropogenic emission reductions in the Atlanta area.

Previous reports on the "Five Cities" study have documented the evaluation of alternative fuel emission scenarios for the New York metropolitan area and the city of St. Louis (Morris et al., 1989a), the use of the UAM to evaluate the effects of biogenic emissions for the Atlanta area (Morris et al., 1989b), and the demonstration of the PLANR use of the UAM for the city of Atlanta and the Dallas-Fort Worth metroplex region (Morris et al., 1989c). This report describes evaluations of PLANR applications of UAM to the St. Louis and Philadelphia regions.

St. Louis

For the application to St. Louis, an ozone episode on 13 July 1976 was selected for modeling. During this period the Regional Air Pollution Study (RAPS) collected data from an intensive measurement network, thus providing a basis for evaluating the PLANR results. Four UAM applications to St. Louis, using different types of inputs, were compared:

UAM(CB-II)	The EPA exercised the 1978-1980 version of the UAM (which incorporates the CB-II chemical mechanism) and its preprocessors using the RAPS data base (Schere and Shreffler, 1982; Cole et al., 1983).
RAPS UAM	The updated UAM (which incorporates CB-IV) was exercised using the RAPS data base. Wind fields, mixing heights, and boundary conditions were prepared using data from RAPS and current UAM preprocessors.
PLANR UAM	The UAM(CB-IV) was exercised using only routinely available meteorological and air quality data and current UAM preprocessors; initial and boundary conditions were assumed to be clean (25 ppbc VOC and 1 ppb NO_x).

SIMPLE UAM	The UAM(CB-IV) was exercised using only RAMMET preprocessed meteorological data (i.e., meteorological observations from a single surface site and mixing heights from the closest upper-air site), resulting in spatially constant winds and mixing heights. Boundary conditions were assumed to be clean.

A comparison of results from these four UAM simulations will provide insight into how data availability affects model performance and how well the model simulates emission control scenarios.

Philadelphia

For the Philadelphia Air Quality Control Region, an ozone episode on 13 July 1979 was selected for modeling. During this period there were several special surface meteorological and air quality monitors in operation as part of the Philadelphia oxidant study (POS). However, since the POS was not in full operation until 18 July 1979, no special upper-air sites were in operation on 13 July 1979.

Considerable effort went into the preparation of input files for the UAM (CB-II) in a past study (Haney and Braverman, 1985). After extensive analysis of the data collected from the POS, several unique interpolation schemes (e.g., urban heat island effects) were used in the preparation of the UAM modeling inputs. These UAM modeling inputs offer a basis for evaluating the PLANR procedures for applying the UAM where only routine data are used in the input preparation. Three different UAM applications to Philadelphia were compared:

UAM(CB-II)	The UAM (CB-II) was exercised using inputs prepared by Systems Applications, Inc. and the EPA using routine data and data from the extensive POS data base (Haney and Braverman, 1985). Initial and boundary conditions were interpolated from all available air quality data.
POS UAM	The UAM (CB-IV) was exercised using the same meteorological inputs as for the UAM (CB-II). Emissions, initial concentrations, and boundary conditions were similar to those used in the UAM (CB-II) run only for the CB-IV chemical mechanism. Routine data and data from the POS were used.
PLANR UAM	Modeling inputs for the UAM (CB-IV) were developed using only routinely available meteorological and air quality data and using current UAM preprocessors.

A comparison of the results from the UAM (CB-II) and POS UAM, which use the same meteorological and air quality inputs, gives a comparison of two different models (the UAM (CB-II) and UAM (CB-IV)) using the same inputs. A comparison of results from the POS UAM and PLANR UAM will give a comparison of two different inputs using the same model (UAM(CB-IV)).

2 DESCRIPTION OF THE CB-IV VERSION OF THE URBAN AIRSHED MODEL

The Urban Airshed Model (UAM) is a three-dimensional grid model designed to calculate the concentrations of both inert and chemically reactive pollutants by simulating the various physical and chemical processes that take place in the atmosphere. The basis of the UAM is the atmospheric diffusion or species continuity equation. This equation represents a mass balance in which all of the relevant emissions, transport, diffusion, chemical reaction, and removal processes are expressed in mathematical terms. Based on the grid concept, the model is generally employed to simulate an 8- to 72-hour period during which episodic meteorological conditions persist.

Because the model can resolve both spatial and temporal features of the concentration field, it is well suited to the analysis of future control strategies and their effects on air quality in various parts of the modeling region. Before the model is used for such an analysis, its ability to replicate measurements from an historical ozone episode is tested. Model inputs are prepared from observed meteorological, emission, and air quality data for a particular day or days. Once the model inputs have been adjusted within the range of their uncertainty so that the model performs within prescribed levels, the emission inventory can be changed to represent assumptions about future emission scenarios. The model is then re-run with the forecasted emissions, and the resulting hourly ozone patterns are what the model predicts is likely to occur under meteorological conditions similar to the historical episode.

The UAM is the only air quality model recommended by the EPA for photochemical or reactive pollutant modeling applications involving entire urban areas (EPA, 1986). The EPA guidelines refer to the 1978-1980 version of the UAM; the formulation of that version is discussed by Ames and others (1985a,b). Many improvements to the UAM have been made over the last 10 years. The two most significant are:

Incorporation of the latest version of the Carbon-Bond Mechanism, the CB-IV (Gery, Whitten, and Killus, 1988)

Use of the Smolarkiewicz algorithm for advection (Smolarkiewicz, 1983)

USE OF THE SMOLARKIEWICZ ALGORITHM TO SOLVE THE ADVECTION EQUATION

Grid-based air quality simulation models require a numerical approximation of the horizontal advection terms in the species conservation equations. The 1978-1980 version of the Urban Airshed Model (UAM) used a variant of the Sharp and Smooth Transport Algorithm (SHASTA) originally formulated by Boris and Book (1973). Since 1977 there have been many comparative studies of advection schemes. Examples of such studies relevant to the UAM are those of Zalesak (1970), Schere (1983), Chock and Dunker (1983), Chock (1985), Smolarkiewicz (1983), and Yamertino and Scire (1985). In each of these studies an idealized scalar function (a cone, block, ellipse, or cosine wave) representative of a concentration distribution is advected by a rotating wind field (constant angular velocity). The rotating wind field provides a range of Courant numbers, depending on the radial distance from the center of the domain. The degree to which the attributes of the idealized function (total mass, peak value, mean value, and gradients) are preserved indicates the accuracy of the scheme.

The above studies showed that a number of advection schemes were more accurate than SHASTA, as measured by the idealized tests. For the UAM, a number of specific requirements constrained the selection of alternative to SHASTA. First, it is important that the scheme be positive definite, i.e., that it not result in negative concentrations. Second, the scheme should use forward time differencing to minimize storage requirements and to insure compatibility with the chemical mechanism numerical solution scheme. Third, the ability of an advection scheme to represent the magnitudes and locations of peak concentrations is of major importance in regulatory applications. Fourth, to handle complex airflows, the scheme should display relatively uniform accuracy over a wide range of Courant numbers (i.e., wind speeds).

Further review indicated that the advection scheme developed by Smolarkiewicz (1983) represented the best combination of accuracy and economy. The Smolarkiewicz scheme is conceptually similar to SHASTA in that a highly diffusive transport step is followed by an anti-diffusive correction step. The transport step is essentially the well-known "upstream" finite-difference scheme. The correction step involves a second exercise of the upstream finite difference scheme, substituting the anti-diffusive velocity for the actual velocity. The Smolarkiewicz scheme is positive definite and forward in time, and can be used in either a time-split or multidimensional mode. Smolarkiewicz demonstrated that the scheme was superior in both accuracy and economy to the multidimensional generalization of SHASTA formulated by Zalesak (1979). In applications to the Los Angeles area and Kern County, California, the UAM with the Smolarkiewicz algorithm produced results that were more accurate than those produced in earlier applications using SHASTA (Hogo, Mahoney, and Yocke, 1988; Whitten et al., 1985).

USE OF THE CB-IV TO SOLVE PHOTOCHEMISTRY

The latest version of the Carbon-Bond Mechanism (CBM-IV) was recently implemented in the UAM (Gery, Whitten, and Killus, 1988). Whenever a new chemical kinetics mechanisms is merged into a complex air quality simulation model, the predictive capabilities and solution speed of the new computer code require optimization and evaluation. This process is even more important now because the recent gas-phase chemical kinetics mechanisms (CAL, RADM, and the CBM-IV) are larger than previous mechanisms, and therefore require significantly more computing time. The CBM-IV reactions are shown in Table 2-1. There are some minor differences between the original CB-IV and the version implemented in the UAM. For the examination of ethanol (ETOH) blended fuels, ETOH was added as a species. The ethanol reaction is $ETOH + OH \rightarrow ALD2 + HO_2$ with a rate constant of 4,300 1/ppm-min. Both numerical and chemical improvements were made to the CB-IV implementation in the UAM so that computational speed could be increased and solution uncertainty diminished.

The implementation of the CB-IV in the UAM used a modified Crank-Nicholson algorithm for the simultaneous solution of the differential equations that represent the chemical changes for each species. This numerical integration scheme produced results that were within a few percent of those obtained with the previous (Gear) algorithm over a wide range of atmospheric conditions (Morris et al., 1989a,c).

TABLE 2-1. The Carbon Bond Mechanism-IV.*

Number	Reaction[1]	Reaction Rate Data		
		Pre-factor (ppm^{-n}min^{-1})	Temp. Factor exp((-E/R)/T)	Rate Constant @ 298K k_{298} (ppm^{-n}min^{-1})
1)	NO2 -hν1-> NO + O			see notes
2)	O -----> O3	8.383 E+04	*EXP(1175/T)	4.323 E+06
3)	O3 + NO -----> NO2	2.643 E+03	*EXP(- 1370/T)	2.664 E+01
4)	O + NO2 -----> NO	1.375 E+04		1.375 E+04
5)	O + NO2 -----> NO3	2.303 E+02	*EXP(687/T)	2.309 E+03
6)	O + NO -----> NO2	3.233 E+02	*EXP(602/T)	2.438 E+03
7)	O3 + NO2 -----> NO3	1.760 E+02	*EXP(- 2450/T)	4.731 E-02
8)	O3 -hν1-> O	5.300 E-02		5.300 E-02×k_1
9)	O3 -hν4-> O1D			see notes
10)	O1D -----> O	1.147 E+05	*EXP(390/T)	4.246 E+05
11)	O1D + H2O -----> 2.00OH	3.260		3.260
12)	O3 + OH -----> HO2	2.344 E+03	*EXP(- 940/T)	1.000 E+02
13)	O3 + HO2 -----> OH	2.100 E+01	*EXP(- 580/T)	2.999
14)	NO3 -hν1-> 0.89NO2 + 0.89O + 0.11NO	3.390 E+01		3.390 E+01×k_1
15)	NO3 + NO -----> 2.00NO2	1.909 E+04	*EXP(250/T)	4.416 E+04
16)	NO3 + NO2 -----> NO + NO2	3.660 E+01	*EXP(- 1230/T)	5.901 E-01
17)	NO3 + NO2 -----> N2O5	7.849 E+02	*EXP(256/T)	1.853 E+03
18)	N2O5 + H2O -----> 2.00HNO3	1.900 E-06		1.900 E-06
19)	N2O5 -----> NO3 + NO2	2.110 E+16	*EXP(-10897/T)	2.776
20)	NO + NO -----> 2.00NO2	2.600 E-05	*EXP(530/T)	1.539 E-04
21)	NO + NO2 + H2O -----> 2.00HONO	1.600 E-11		1.600 E-11
22)	OH + NO -----> HONO	6.554 E+02	*EXP(806/T)	9.799 E+03
23)	HONO -hν1-> OH + NO	1.975 E-01		1.975 E-01×k_1
24)	OH + HONO -----> NO2	9.770 E+03		9.770 E+03
25)	HONO + HONO -----> NO + NO2	1.500 E-05		1.500 E-05
26)	OH + NO2 -----> HNO3	1.537 E+03	*EXP(713/T)	1.682 E+04
27)	OH + HNO3 -----> NO3	7.600	*EXP(1000/T)	2.179 E+02
28)	HO2 + NO -----> OH + NO2	5.482 E+03	*EXP(240/T)	1.227 E+04
29)	HO2 + NO2 -----> PNA	1.640 E+02	*EXP(749/T)	2.025 E+03
30)	PNA -----> HO2 + NO2	2.876 E+15	*EXP(-10121/T)	5.115
31)	OH + PNA -----> NO2	1.909 E+03	*EXP(380/T)	6.833 E+03
32)	HO2 + HO2 -----> H2O2	8.739 E+01	*EXP(1150/T)	4.144 E+03
33)	HO2 + HO2 + H2O -----> H2O2	7.690 E-10	*EXP(5800/T)	2.181 E-01
34)	H2O2 -hν3-> 2.00OH	2.550 E-01		2.550 E-01×k_{39}
35)	OH + H2O2 -----> HO2	4.720 E+03	*EXP(- 187/T)	2.520 E+03
36)	OH + CO -----> HO2	3.220 E+02		3.220 E+02
37)	FORM + OH -----> HO2 + CO	1.500 E+04		1.500 E+04
38)	FORM -hν2-> CO + 2.00HO2			see notes
39)	FORM -hν3-> CO			see notes
40)	FORM + O -----> OH + HO2 + CO	4.302 E+04	*EXP(- 1550/T)	2.370 E+02
41)	FORM + NO3 -----> HNO3 + HO2 + CO	9.300 E-01		9.300 E-01
42)	ALD2 + O -----> C2O3 + OH	1.739 E+04	*EXP(- 986/T)	6.360 E+02
43)	ALD2 + OH -----> C2O3	1.037 E+04	*EXP(250/T)	2.400 E+04
44)	ALD2 + NO3 -----> C2O3 + HNO3	3.700		3.700
45)	ALD2 -hν6-> FORM + XO2 + CO + 2.00HO2			see notes
46)	C2O3 + NO -----> NO2 + XO2 + FORM + HO2	7.915 E+03	*EXP(250/T)	1.831 E+04
47)	C2O3 + NO2 -----> PAN	1.180 E-04	*EXP(5500/T)	1.223 E+04
48)	PAN -----> C2O3 + NO2	5.616 E+18	*EXP(-14000/T)	2.220 E-02
49)	C2O3 + C2O3 -----> 2.00FORM + 2.00XO2 + 2.00HO2	3.700 E+03		3.700 E+03
50)	C2O3 + HO2 -----> 0.79FORM + 0.79XO2 + 0.79HO2 + 0.79OH	9.600 E+03		9.600 E+03
51)	OH -----> XO2 + FORM + HO2	6.521 E+03	*EXP(- 1710/T)	2.100 E+01

(Continued)

*As currently implemented in the UAM (CB-IV), isoprene is not explicitly treated as a separate species, and ethanol has been added to the CB-IV.

89092
87048r
88097
88151

TABLE 2-1 Concluded.

Number	Reaction[1]	Reaction Rate Data		
		Pre-factor ($ppm^{-n}min^{-1}$)	Temp. Factor exp((-E/R)/T)	Rate Constant @ 298K k_{298} ($ppm^{-n}min^{-1}$)
52)	PAR + OH -----> 0.87XO2 + 0.13XO2N + 0.11HO2 + 0.11ALD2 + 0.76ROR - 0.11PAR	1.203 E+03		1.203 E+03
53)	ROR -----> 1.10ALD2 + 0.96XO2 + 0.94HO2 + 0.04XO2N + 0.02ROR - 2.10PAR	6.250 E+16	*EXP(- 8000/T)	1.371 E+05
54)	ROR -----> HO2	9.545 E+04		9.545 E+04
55)	ROR + NO2 ----->	2.200 E+04		2.200 E+04
56)	O + OLE -----> 0.63ALD2 + 0.38HO2 + 0.28XO2 + 0.30CO + 0.20FORM + 0.02XO2N + 0.22PAR + 0.20OH	1.756 E+04	*EXP(- 324/T)	5.920 E+03
57)	OH + OLE -----> FORM + ALD2 + XO2 + HO2 - PAR	7.740 E+03	*EXP(504/T)	4.200 E+04
58)	O3 + OLE -----> 0.50ALD2 + 0.74FORM + 0.33CO + 0.44HO2 + 0.22XO2 + 0.10OH - PAR	2.104 E+01	*EXP(- 2105/T)	1.800 E-02
59)	NO3 + OLE -----> 0.91XO2 + FORM + ALD2 + 0.09XO2N + NO2 - PAR	1.135 E+01		1.135 E+01
60)	O + ETH -----> FORM + 0.70XO2 + CO + 1.70HO2 + 0.30OH	1.540 E+04	*EXP(- 792/T)	1.080 E+03
61)	OH + ETH -----> XO2 + 1.56FORM + HO2 + 0.22ALD2	3.000 E+03	*EXP(411/T)	1.192 E+04
62)	O3 + ETH -----> FORM + 0.42CO + 0.12HO2	1.856 E+01	*EXP(- 2633/T)	2.700 E-03
63)	OH + TOL -----> 0.08XO2 + 0.36CRES + 0.44HO2 + 0.56TO2	3.106 E+03	*EXP(322/T)	9.150 E+03
64)	TO2 + NO -----> 0.90NO2 + 0.90HO2 + 0.90OPEN	1.200 E+04		1.200 E+04
65)	TO2 -----> CRES + HO2	2.500 E+02		2.500 E+02
66)	OH + CRES -----> 0.40CRO + 0.60XO2 + 0.60HO2 + 0.30OPEN	6.100 E+04		6.100 E+04
67)	CRES + NO3 -----> CRO + HNO3	3.250 E+04		3.250 E+04
68)	CRO + NO2 ----->	2.000 E+04		2.000 E+04
69)	OPEN -hν2-> C2O3 + HO2 + CO	9.040		9.040 $*k_{38}$
70)	OPEN + OH -----> XO2 + 2.00CO + 2.00HO2 + C2O3 + FORM	4.400 E+04		4.400 E+04
71)	OPEN + O3 -----> 0.03ALD2 + 0.62C2O3 + 0.70FORM + 0.03XO2 + 0.69CO + 0.08OH + 0.76HO2 + 0.20MGLY	8.030 E-02	*EXP(- 500/T)	1.500 E-02
72)	OH + XYL -----> 0.70HO2 + 0.50XO2 + 0.20CRES + 0.80MGLY + 1.10PAR + 0.30TO2	2.453 E+04	*EXP(116/T)	3.620 E+04
73)	OH + MGLY -----> XO2 + C2O3	2.600 E+04		2.600 E+04
74)	MGLY -hν2-> C2O3 + HO2 + CO	9.640		9.640 $*k_{38}$
75)	O + ISOP -----> 0.60HO2 + 0.80ALD2 + 0.55OLE + 0.50XO2 + 0.50CO + 0.45ETH + 0.90PAR	2.700 E+04		2.700 E+04
76)	OH + ISOP -----> XO2 + FORM + 0.67HO2 + 0.40MGLY + 0.20C2O3 + 1.00ETH + 0.20ALD2 + 0.13XO2N	1.420 E+05		1.420 E+05
77)	O3 + ISOP -----> FORM + 0.40ALD2 + 0.55ETH + 0.20MGLY + 0.10PAR + 0.06CO + 0.44HO2 + 0.10OH	1.800 E-02		1.800 E-02
78)	NO3 + ISOP -----> XO2N	4.700 E+02		4.700 E+02
79)	XO2 + NO -----> NO2	1.200 E+04		1.200 E+04
80)	XO2 + XO2 ----->	2.550 E+01	*EXP(1300/T)	2.000 E+03
81)	XO2N + NO ----->	1.000 E+03		1.000 E+03

89092

87048r 11

88097
88151

3 DEVELOPMENT OF A PLANR UAM BASE CASE FOR ST. LOUIS

DEFINITION OF THE PLANR BASE CASE

One of the key components of the PLANR use of the UAM is a limitation on the number of diagnostic simulations used to arrive at a base case. This is achieved by relaxing the strict model performance standards expected of the UAM in the past. Although the goal is to achieve a satisfactory level of performance with as few diagnostic simulations as possible, the model must show some skill in predicting ozone observations in order to have confidence that the model will respond properly to changes in emissions.

The minimal performance goal in the past was to have the predicted regional maximum ozone concentration be within 30 percent and in the general location of the peak observed value. Model performance has been considered good if the predicted peak ozone is within 15 percent. Clearly, when model inputs are based only on sparse routine data, rather than intensively measured data as in the past, model performance cannot be expected to always be as good in the past. However, there should be some minimal expectations of model performance since incorrect characterization of base case ozone concentrations may lead to incorrect calculations of ozone reductions due to alternative emission inputs.

The protocols for several recent UAM studies of the impacts of California offshore drilling emissions (Haney et al., 1986; Yocke et al., 1985) defined a minimal model performance standard as follows: (1) the UAM-predicted regional maximum ozone concentration should be within 20 percent and in the general location of the observed maximum, and (2) the UAM predicted maximum at the location of the observed maximum should be within 30 percent of the observed value.

We adopted this model performance standard for the PLANR use of the UAM for St. Louis. It should be emphasized, however, model evaluation should always address the issue of whether the right answer is being obtained for the right reason.

METEOROLOGICAL CONDITIONS

The ozone episode on 13 July 1976 was chosen as the base case. During the early morning hours on 13 July a weak warm front extended across the Upper Mississippi

Valley through southwestern Iowa and across central Missouri. This is illustrated in the daily weather map depicted in Figure 3-1. To the northeast of the warm front a high pressure system was slowly moving eastward. Circulation about the high-pressure system, which extended to the St. Louis area, was from the northeast during the morning hours (see Figure 3-2, the 950 mb map at 0600 CST). The winds became more southeasterly as the high pressure to the north moved eastward (see Figure 3-3, the 950 mb map at 0600 CST). An examination of the surface winds at Lambert Field reveals a significant wind shift from the northeast to the west at around 1130 CST, marking the passage of the warm front through St. Louis. Surface winds at Lambert Field remained out of the west to southwest the remainder of the day. By 0600 CST the warm front had passed St. Louis but had not yet reached Salem, IL (see Figure 3-3). Thus it appears on 13 July 1976 that air parcels originating early in the morning at St. Louis would travel west of St. Louis, but then come back over the city later in the afternoon.

PREPARATION OF INPUTS

An important component of the PLANR use of the UAM is consistency in the procedures used to prepare model inputs for different cities. Procedures to be followed in preparing UAM inputs from limited data must be flexible. These procedures are currently being refined and evaluated to determine the optimum methodologies for generating UAM inputs from limited data.

The preprocessor programs supplied with the 1978-1980 version of the UAM generally rely on intensively measured data; the additional data needed to obtain gridded fields of input parameters for the UAM are interpolated from these measurements. Over the last 10 years many of these programs have become outdated. More recent applications of the UAM have prepared input data using techniques that have been developed on a case-by-case basis and are tailored to the available data. In the following paragraphs we discuss the procedures used to prepare meteorological and air quality inputs for the PLANR study of St. Louis.

Data Availability

Routine data collection in or near St. Louis for 13 July 1976 consists of six surface meteorological observation sites located at airports (i.e., Federal Aviation Administration sites) surrounding St. Louis (see Figure 3-4). There were no routine air quality or upper-air measurement sites. For the PLANR application of UAM to St. Louis, data from the six surface sites were used along with twice-daily upper-air observations from two sites outside of St. Louis: Salem IL, approximately 120 km east of St. Louis, and Monett, MO, approximately 340 km west-southwest of St. Louis. Since only routine data are being used, transport conditions in this area may be incorrectly characterized because of the absence of surface meteorological data within the urban core.

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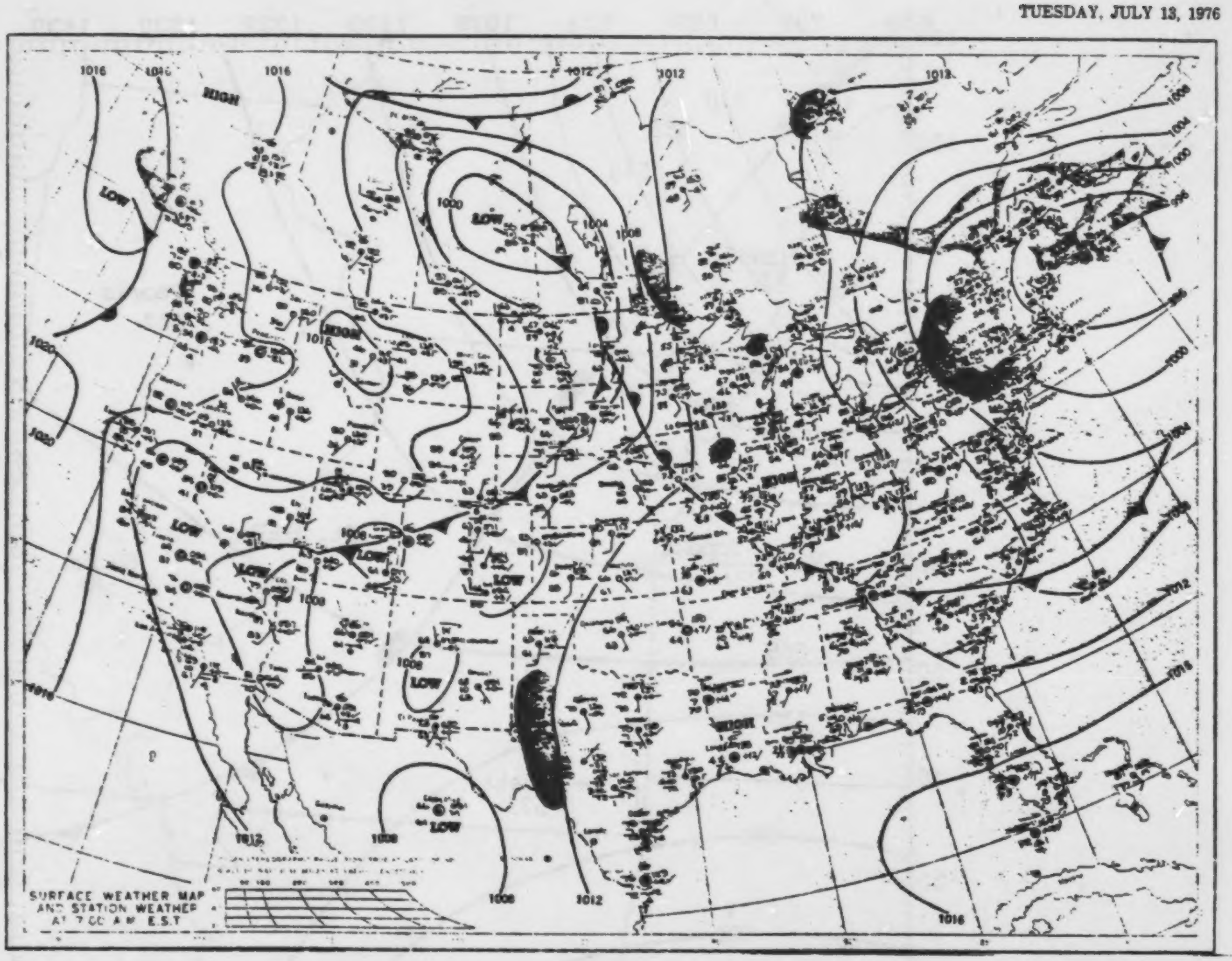

TUESDAY, JULY 13, 1976
SURFACE WEATHER MAP AND STATION WEATHER AT 7:00 A.M. E.S.T.
HIGH
LOW
HIGH
LOW
LOW
LOW
LOW
LOW
LOW
HIGH
LOW
HIGH
1016
1016
1016
1012
1012
1012
1008
1004
1000
996
1000
1004
1008
1012
1016
1020
1020
1016
1012
1008
1008
1012
1016

FIGURE 3-1. Surface weather map at 0700 EST on 13 July 1976.

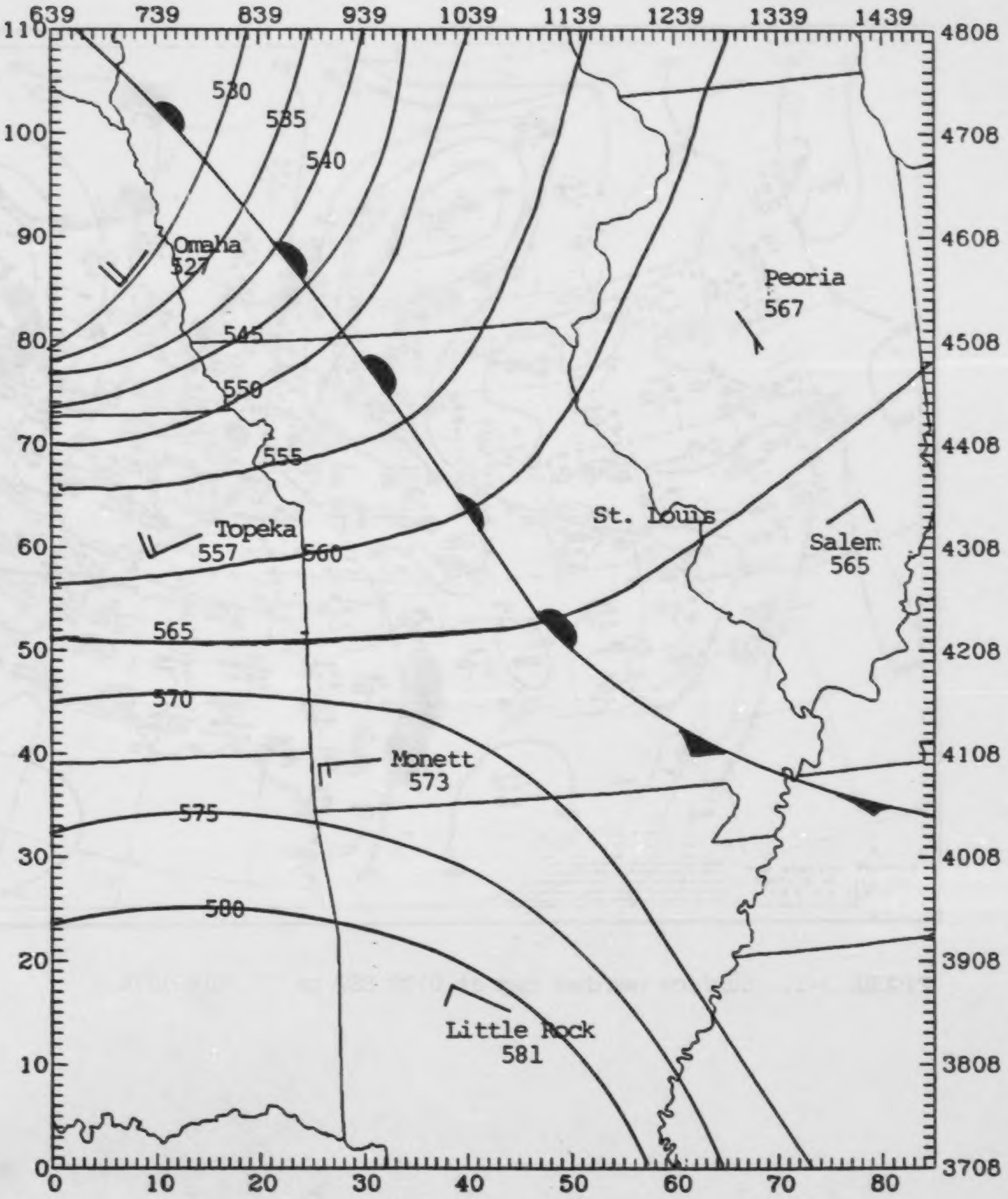
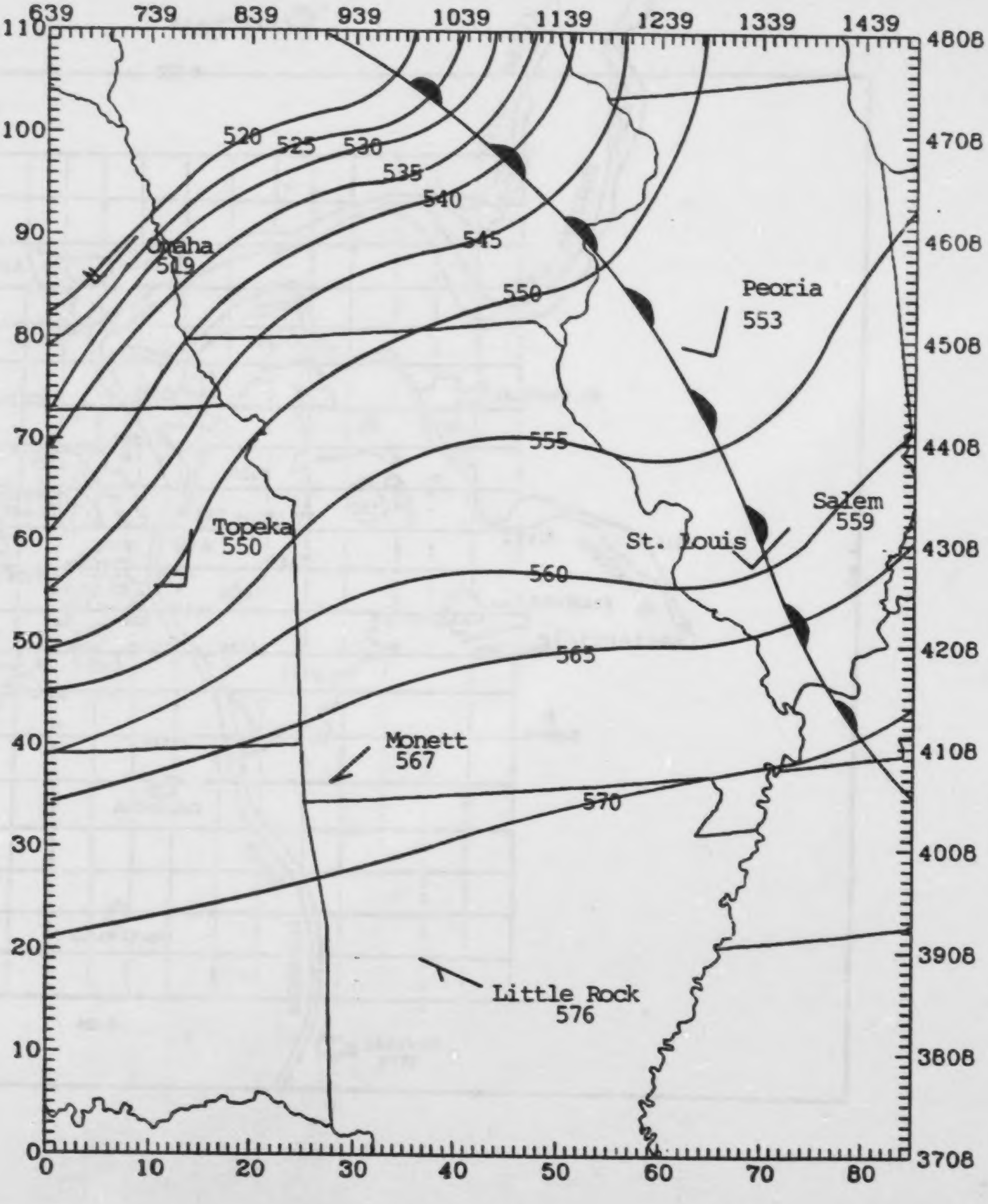

639
739
839
939
1039
1139
1239
1339
1439
110
100
90
80
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70
80
4808
4708
4608
4508
4408
4308
4208
4108
4008
3908
3808
3708
530
535
540
545
550
555
560
565
570
575
580
Omaha
527
Topeka
557
Monett
573
Little Rock
581
St. Louis
Peoria
567
Salem
565

FIGURE 3-2. 950 millibar constant pressure surface in the vicinity of St. Louis at 1800 LST 13 July 1976 showing 950 mb heights (m msl) and winds.


639
739
839
939
1039
1139
1239
1339
1439
110
100
90
80
70
60
50
40
30
20
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0
0
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30
40
50
60
70
80
4808
4708
4608
4508
4408
4308
4208
4108
4008
3908
3808
3708
520
525
530
535
540
545
550
555
560
565
570
Omaha
519
Peoria
553
Topeka
550
St. Louis
Salem
559
Monett
567
Little Rock
576

FIGURE 3-3. 950 millibar constant pressure surface in the vicinity of St. Louis at 1800 LST 14 July 1976 showing 950 mb heights (m msl) and winds.

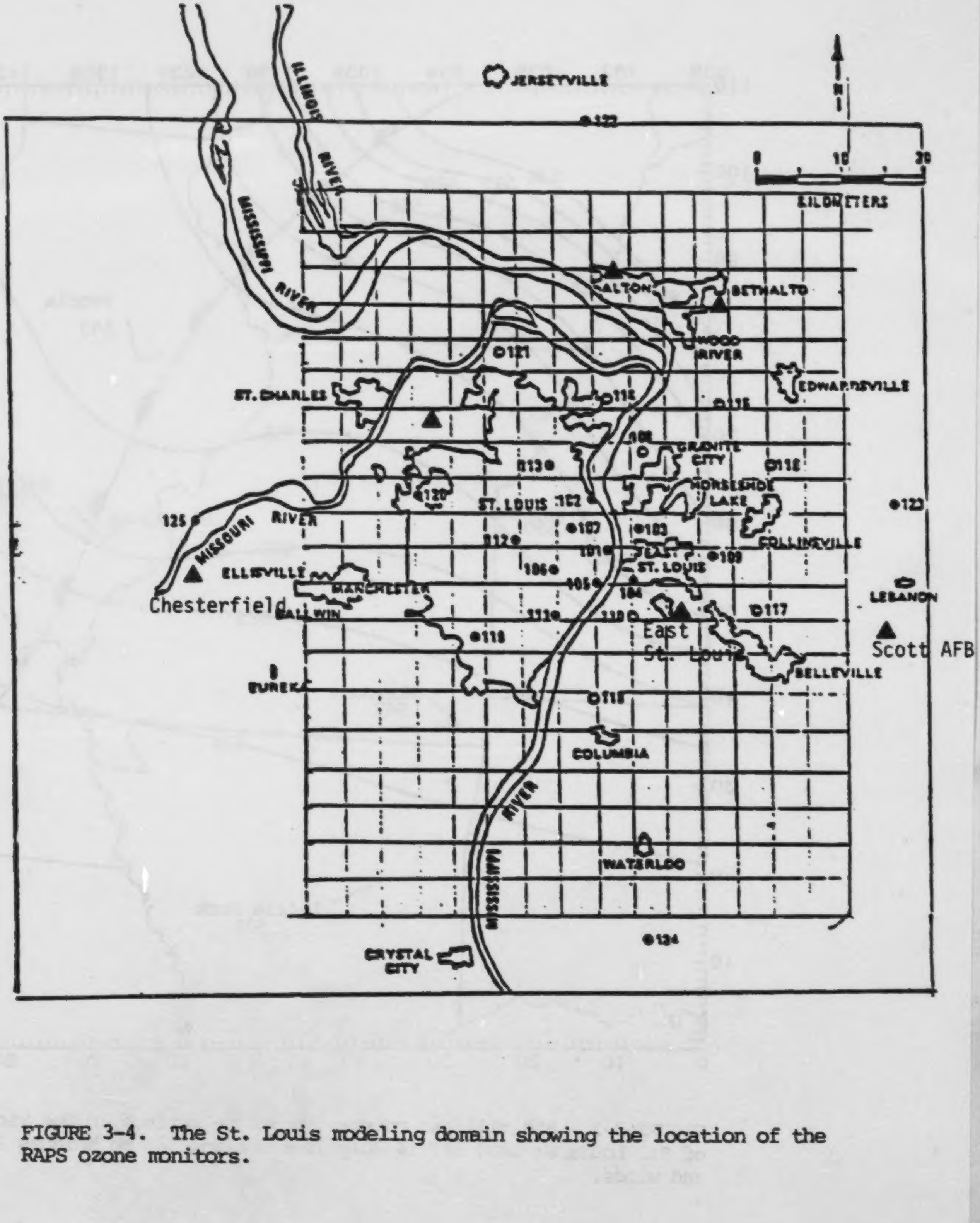

JERSEYVILLE
122
ILLINOIS RIVER
MISSISSIPPI RIVER
N
0
10
20
KILOMETERS
ALTON
BETHALTO
WOOD RIVER
121
EDWARDSVILLE
ST. CHARLES
114
115
108
GRANITE CITY
113
116
HORSESHOE LAKE
120
ST. LOUIS
102
123
125
MISSOURI RIVER
107
103
COLLINSVILLE
112
101
EAST ST. LOUIS
109
ELLISVILLE
106
105
104
LEBANON
Chesterfield
MANCHESTER
BALLWIN
111
110
117
East St. Louis
Scott AFB
118
BELLEVILLE
EUREKA
119
COLUMBIA
MISSISSIPPI RIVER
WATERLOO
124
CRYSTAL CITY

FIGURE 3-4. The St. Louis modeling domain showing the location of the RAPS ozone monitors.

Wind Field Preprocessor

One of the most important UAM inputs is the wind field. A key component in the PLANR use of the UAM will be use of the Diagnostic Wind Model developed by Systems Applications, Inc. for the EPA (Douglas and Kessler, 1988). This model was developed to calculate wind fields for regions of complex terrain for which wind data were sparse (Morris et al., 1987, 1988).

The DWM was used to generate hourly gridded wind fields for both the PLANR and RAPS UAM simulations. This model incorporates local surface and upper-air observations, where available, and provides some information on terrain-induced airflow in regions where local observations are unavailable. The DWM is formulated in terrain-parallel coordinates. Wind fields are generated in a two-step procedure.

In Step 1, a domain-mean wind, which is obtained from a representative upper-air observation, is adjusted for terrain effects. These include the kinematic effects of terrain (the lifting and acceleration of the airflow over terrain obstacles), thermodynamically generated slope flows, and blocking effects. Step 1 produces a spatially varying gridded field of u and v for each vertical layer within the model domain. Defining the most representative hourly upper-air sounding from twice a day upper-air observations from the routine NWS network is a critical step of the PLANR use of the UAM. As will be seen, this usually requires interpretation of the meteorological conditions of the modeling period.

In Step 2, observational information is added to the Step 1 (u,v) field. Using an objective analysis procedure, observations are used within a user-specified radius of influence while the Step 1 (u,v) field dominates in subregions where observations are unavailable. This procedure consists of four substeps: (1) interpolation, (2) smoothing of the analyzed field, (3) computation of a vertical velocity field, and (4) minimization of the three-dimensional divergence. The following modified inverse-distance-squared weighting scheme (Ross and Smith, 1986) is used for the interpolation:

$$(u,v)' = \{ \sum_k [r_k^{-2}(u_o,v_o)_k] + R^{-2}(u,v)_1 \} / \{ \sum_k r_k^{-2} + R^{-2} \}$$

where $(u_o,v_o)_k$ denotes an observed wind at station k, r_k is the distance from station k to a given grid point, $(u,v)_1$ is the Step 1 wind field, and $(u,v)'$ is the updated wind vector. The radius R determines whether observations or the Step 1 wind field will be used.

Following the interpolation, a five-point smoother is applied to the analyzed wind field to reduce discontinuities that may result from the interpolation. An initial vertical velocity, W', is calculated from $(u,v)'$ by integrating the incompressible conservation-of-mass equation. It has been noted that vertical velocities obtained from an objectively anlayzed field may be unrealistically large near the top of the domain (Godden and Lurmann, 1983). In the DWM, W' is modified using a procedure suggested by O'Brien (1970):

$$W_2(Z) = W'(Z) - (Z/Z_{top})W'_{top}$$

where Z is the height in terrain-following coordinates and Z_{top} is the height of the model top. Note that W_2 is zero at the top of the model.

After the vertical velocity profile is adjusted, it is necessary to adjust the objective analysis product (u,v)' so that it is mass-consistent with W_2. An iterative adjustment of the horizontal (u,v) field is performed to minimize the three-dimensional divergence within each layer. The adjusted horizontal wind field $(u,v)_2$ is the final product of the diagnostic model.

For both the PLANR and RAPS UAM applications to St. Louis the DWM was exercised with 13 to 14 vertical levels using available meteorological measurements. These wind fields were then vertically averaged to the five vertical layers used in the UAM applications. The differences in the PLANR and RAPS wind fields were in the amount and frequency of surface and upper-air data used.

Model Inputs

The following paragraphs describe how the 10 main UAM input files were prepared for the PLANR application of the UAM to St. Louis.

DIFFBREAK: This file contains the daytime mixing height or nighttime inversion height for each column of cells at the beginning and end of each hour of the simulation. Hourly mixing heights were estimated at five routine surface meteorological sites through use of the hourly surface measurements of temperature and the twice daily upper-air observations from a representative upper-air site using the RAMMET meteorological preprocessor. The resultant hourly mixing heights at each of the surface sites were then spatially interpolated using the UAM preprocessor program DFSNBK specifying the 1/r interpolation option.

Due to the presence of a warm front to the east of St. Louis in the afternoon that separated St. Louis from Salem, IL the Monett MO upper-air observations were used to define the mixing heights for all of the PLANR evaluation runs. The wind and temperature observations over Monett were thought to be more representative of the air over St. Louis despite the fact that the Salem upper-air site is closer to St. Louis (120 km) than is Monett, MO (340 km). The maximum daily mixing height produced using the Monett upper-air observations and St. Louis surface observations was approximately 1,950 m agl. Note that the Salem IL, upper-air sounding produced a maximum daily mixing height of 2,350 m agl.

REGIONTOP: This file contains the height of each column of cells at the beginning and end of each hour of the simulation. If this height is greater than the mixing height, the cell or cells above the mixing height are assumed to be within an inversion. For the PLANR study of St. Louis a constant 2,000 m agl region top was used. This value was picked because it is 50 meters above the maximum mixing height. Thus all five vertical layers of the UAM are contained within the well mixed layer, offering the maximum vertical resolution possible with the five-layer configuration.

WIND: This file contains the x and y components of the wind velocity for every grid cell for each hour of the simulation. There are two steps in creating the wind fields for St. Louis: (1) exercising the Diagnostic Wind Model (DWM) using 14 vertical levels and data from the six routine surface and a representative upper-air meteorological observation sites; and (2) vertical interpolation of the 15-layer hourly wind fields into the five layers used in this application. As noted above, the main difference between the three diagnostic runs was in the wind inputs into the DWM, namely the definition of the representative upper-air sounding, and, in run #3 the magnitudes of the surface wind observations were changed.

METSCALARS: This file contains the hourly values of the meteorological parameters that do not vary spatially. These scalars are the NO_2 photolysis rate constant, the concentration of water vapor, the temperature gradient above and below the inversion base, atmospheric pressure, and exposure class. The NO_2 photolysis rates were calculated for the CB-IV mechanism using procedures described by Schere and Demerjian (1977) and actinic flux data collected by Bass and coworkers (Bass et al., 1980; Gery, Whitten, and Killus, 1988). The concentration of water was based on measurements of temperature and dew point at the surface meteorological observation sites. The observed water concentrations at all of the surface sites were averaged to obtain the hourly input for the UAM. Exposure class was assigned based on the solar intensity: a value of -2 at night; and daytime values of either 0 (one hour day/night transition period) to 3. The temperature gradients below the inversion (TGRADBELOW) and above (TGRADABOVE) were based on the twice-daily upper-air soundings at Monett, MO.

AIRQUALITY: This file contains the initial concentrations of each species for each grid cell at the start of the simulation. For the PLANR study of St. Louis we used the following "clean values" for initial concentrations for all diagnostic simulations:

VOC = 25 ppbc (using EKMA default speciation)
ISOP = 0.001 ppb
NO_x = 1 ppb (3/4 NO_2, 1/4 NO)
O_3 = 40 ppb
CO = 200 ppb

BOUNDARY and TOPCONC: These files define the location of the modeling region boundaries and specify the concentration of each species that is used as the boundary condition along each boundary at each vertical level and above the region top. For the PLANR study of St. Louis, the clean values listed above were used for boundary conditions.

TEMPERATUR: This file contains the hourly temperature for each surface layer grid cell. Hourly spatial varying temperatures were obtained by using 1/r interpolation from the surface meteorlogical observations.

EMISSIONS and **PTSOURCE:** The original area and point source emissions inventories used in UAM/CB-II simulations (Schere and Shreffler, 1982) were converted to correspond with the CB-IV mechanism. The conversions are described in Table 3-1.

DIAGNOSTIC SIMULATIONS TO ARRIVE AT A BASE CASE

The PLANR use of the UAM limits the number of diagnostic simulations, which are designed to improve model performance for a particular application to an acceptable level. Many past UAM applications involved several diagnostic simulations. Diagnostic simulations usually involve varying uncertain inputs, such as wind fields and mixing heights, within their ranges of uncertainties. For the PLANR use of the UAM the number of diagnostic simulations is limited, and the most representative simulation is used as a base case for modeling analyses of control scenarios.

For St. Louis, three diagnostic simulations were performed before an acceptable base case was achieved. The three simulations differed in how the observed surface and upper-air meteorological observations were interpolated and adjusted in the UAM preprocessor. In the PLANR use of UAM for Atlanta, four diagnostic simulations were needed (Morris et al., 1989b).

The three diagnostic simulations for the PLANR UAM study of St. Louis differed as follows:

> **Diagnostic Run #1:** Because of the warm front between St. Louis and Salem on the afternoon of 13 July, the upper-air soundings from Monett, MO were believed to be more representative of the air over St. Louis than those from Salem, IL. Thus the Monett upper-air observations were used to define the mixing heights and domain-mean wind input into the DWM. The twice-daily upper-air wind observations were linearly interpolated to the hour in question for input into the DWM. Other meteorological observations (e.g. surface winds and temperatures) were used with no adjustments.
>
> **Diagnostic Run #2:** An examination the surface wind observations indicated that the warm front passes through St. Louis around noon. Thus the Salem upper-air sounding at 0600 LST was used as input into the DWM until noon; a

TABLE 3-1. Respeciation of emissions of hydrocarbons.

CBM-IV Species	As a Function of CBM-II Species
OLE	OLE
PAR	PAR - ARO * 0.432 - ARO * 2 * 0.568
TOL	ARO * 0.432
XYL	ARO * 0.568
FORM	CARB * 0.288
ALD2	CARB * 0.712
ETH	ETH
CRES	1 X 10^{-6} ppm
MGLY	1 X 10^{-6} ppm
OPEN	1 X 10^{-6} ppm

linear interpolation of the Monett soundings at 0600 and 1800 LST was used for the afternoon. Mixing heights were defined from the Monett upper-air sounding and the surface temperature observations.

Diagnostic Run #3: It has been noted in studies in the South Coast Air Basin that hourly averged wind observations and collocated NWS or FAA instantaneous wind observations generally do not agree. During periods of stagnation and low wind speeds, the hourly surface wind speeds reported by the NWS or FAA tend to have a positive bias, generally 1 to 2 times the values reported by the hourly averged monitors. Therefore, in this diagnostic run all FAA surface wind speed observations were reduced by 50 percent for input into the DWM. Other inputs remained as in diagnostic run 2.

Diagnostic Run 1

In the first diagnostic run, the meteorological observations were used with no adjustments in the UAM preprocessors. Observations from Monett, MO were chosen as the representative upper-air sounding for calculating mixing heights and the domain-mean wind input for the DWM. Figure 3-5 shows isopleths of the predicted maximum daily ozone concentrations along with the daily maximum observations. The predicted region-wide maximum ozone concentration for diagnostic run 1 is 16.2 pphm, compared to the observed maximum of 22.2 pphm, and occurs approximately 20 km north-northeast of the observed maximum. The predicted region-wide maximum ozone concentration is within 27 percent of the observed maximum when the two are compared unmatched by location or hour. The predicted maximum ozone concentration at the location of the observed maximum was half (11.1 pphm) of the observed peak (22.2 pphm).

An examination of Figure 3-5 reveals two reasons why run #1 is not an acceptable base case: (1) model performance is poor (the predicted region-wide peak ozone is only within 27 percent of the observed peak, and at the location of the observed peak the predicted peak is within only 50 percent) and (2) the predicted region-wide peak ozone occurs too close to the boundary. Reducing VOC emissions in this run would tend to move the predicted peak ozone concentrations further downwind. It is very likely the model would locate this peak ozone outside of the modeling domain if the run 1 inputs were used, resulting in incorrect ozone reductions.

Diagnostic Run 2

As noted previously, a warm front passes through St. Louis around noon on 13 July 1976. Thus the upper-air sounding at Salem, IL is more representative of the air over St. Louis in the morning, whereas in the afternoon, after the warm front moves to the east of St. Louis, the upper-air sounding at Monett is more representative. For

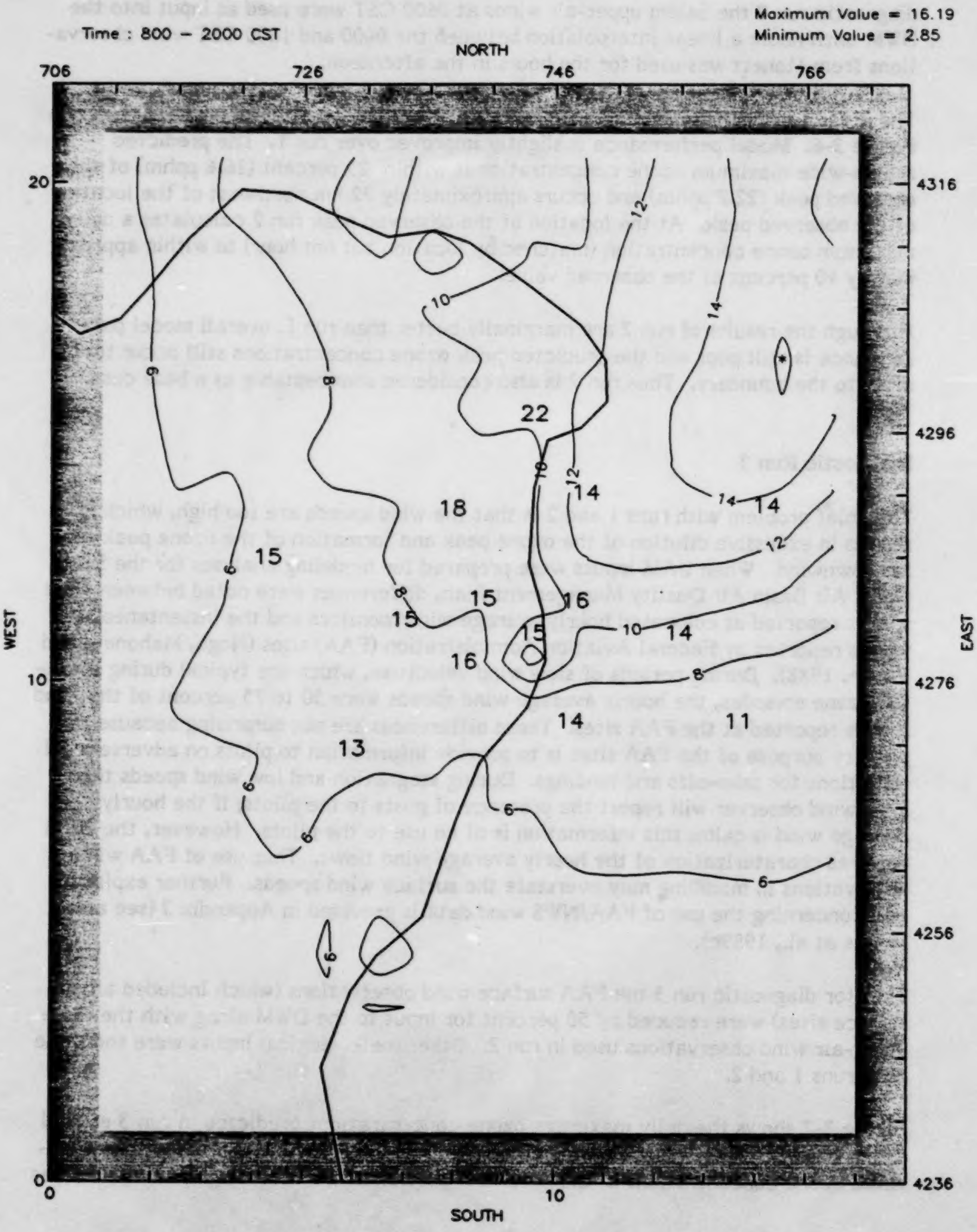

Time : 800 – 2000 CST
Maximum Value = 16.19
Minimum Value = 2.85
NORTH
706
726
746
766
20
10
0
4316
4296
4276
4256
4236
0
10
SOUTH
WEST
EAST
10
12
14
9
8
22
10
12
14
14
14
18
15
15
15
16
15
14
10
12
16
8
14
11
13
6
6
6
6
9
6

FIGURE 3-5. Isopleths of predicted maximum daily ozone concentrations (pphm) with superimposed maximum daily observations for PLANR diagnostic run #1.

diagnostic run 2 the Salem upper-air winds at 0600 CST were used as input into the DWM until noon; a linear interpolation between the 0600 and 1800 CST wind observations from Monett was used for the hours in the afternoon.

The predicted daily maximum ozone concentrations for diagnostic run 2 are shown in Figure 3-6. Model performance is slightly improved over run 1. The predicted region-wide maximum ozone concentration is within 25 percent (16.6 pphm) of the observed peak (22.2 pphm) and occurs approximately 22 km northeast of the location of the observed peak. At the location of the observed peak run 2 calculates a daily maximum ozone concentration (matched by location but not hour) to within approximately 40 percent of the observed value.

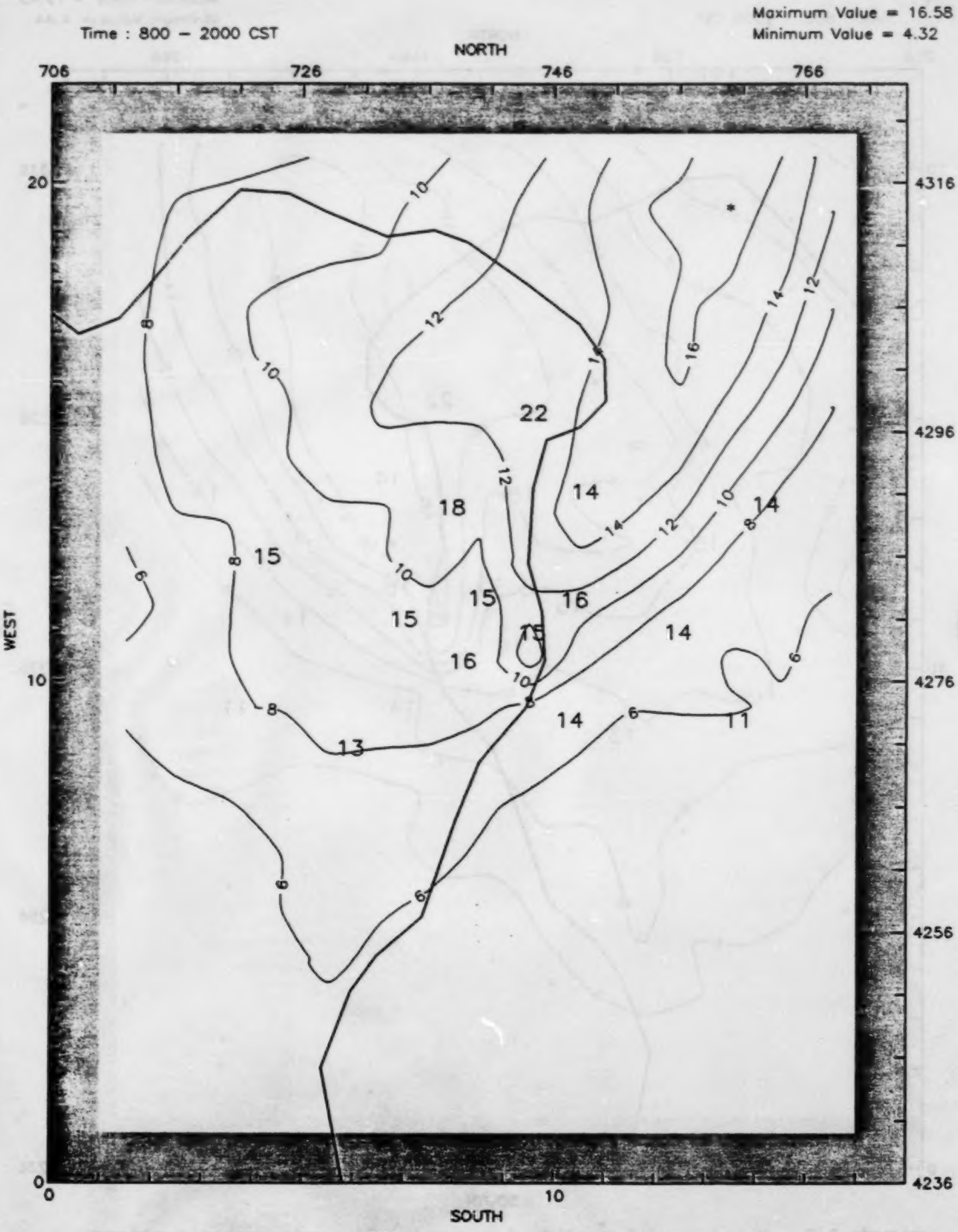
Although the results of run 2 are marginally better than run 1, overall model performance is still poor and the predicted peak ozone concentrations still occur too close to the boundary. Thus run 2 is also considered unacceptable as a base case.

Diagnostic Run 3

The chief problem with runs 1 and 2 is that the wind speeds are too high, which results in excessive dilution of the ozone peak and formation of the ozone peak too far downwind. When UAM inputs were prepared for modeling analyses for the South Coast Air Basin Air Quality Management Plan, differences were noted between wind speeds reported at colocated hourly average wind monitors and the instantaneous values reported by Federal Aviation Administration (FAA) sites (Hogo, Mahoney, and Yocke, 1988). During periods of slow wind velocities, which are typical during elevated ozone episodes, the hourly average wind speeds were 50 to 75 percent of the wind speeds reported at the FAA sites. These differences are not surprising because the primary purpose of the FAA sites is to provide information to pilots on adverse wind conditions for take-offs and landings. During stagnation and low wind speeds the FAA wind observer will report the presence of gusts to the pilots; if the hourly average wind is calm, this information is of no use to the pilots. However, the UAM requires charaterization of the hourly average wind flows. Thus use of FAA wind observations in modeling may overstate the surface wind speeds. Further explanation concerning the use of FAA/NWS wind data is provided in Appendix J (see also Morris et al., 1989c).

Thus for diagnostic run 3 the FAA surface wind observations (which included all six surface sites) were reduced by 50 percent for input to the DWM along with the same upper-air wind observations used in run 2. Other meteorlogical inputs were the same as in runs 1 and 2.

Figure 3-7 shows the daily maximum ozone concentrations predicted in run 3 as well as the observed daily maximums. In runs 1 and 2 the UAM predicted a region of elevated ozone concentrations in the northeast portion of the modeling domain, whereas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Maximum Value = 16.58
Minimum Value = 4.32
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746
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SOUTH
0
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WEST
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10
0
EAST
4316
4296
4276
4256
4236
22
18
15
15
15
15
16
16
14
14
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14
13
11
6
6
6
8
8
8
8
10
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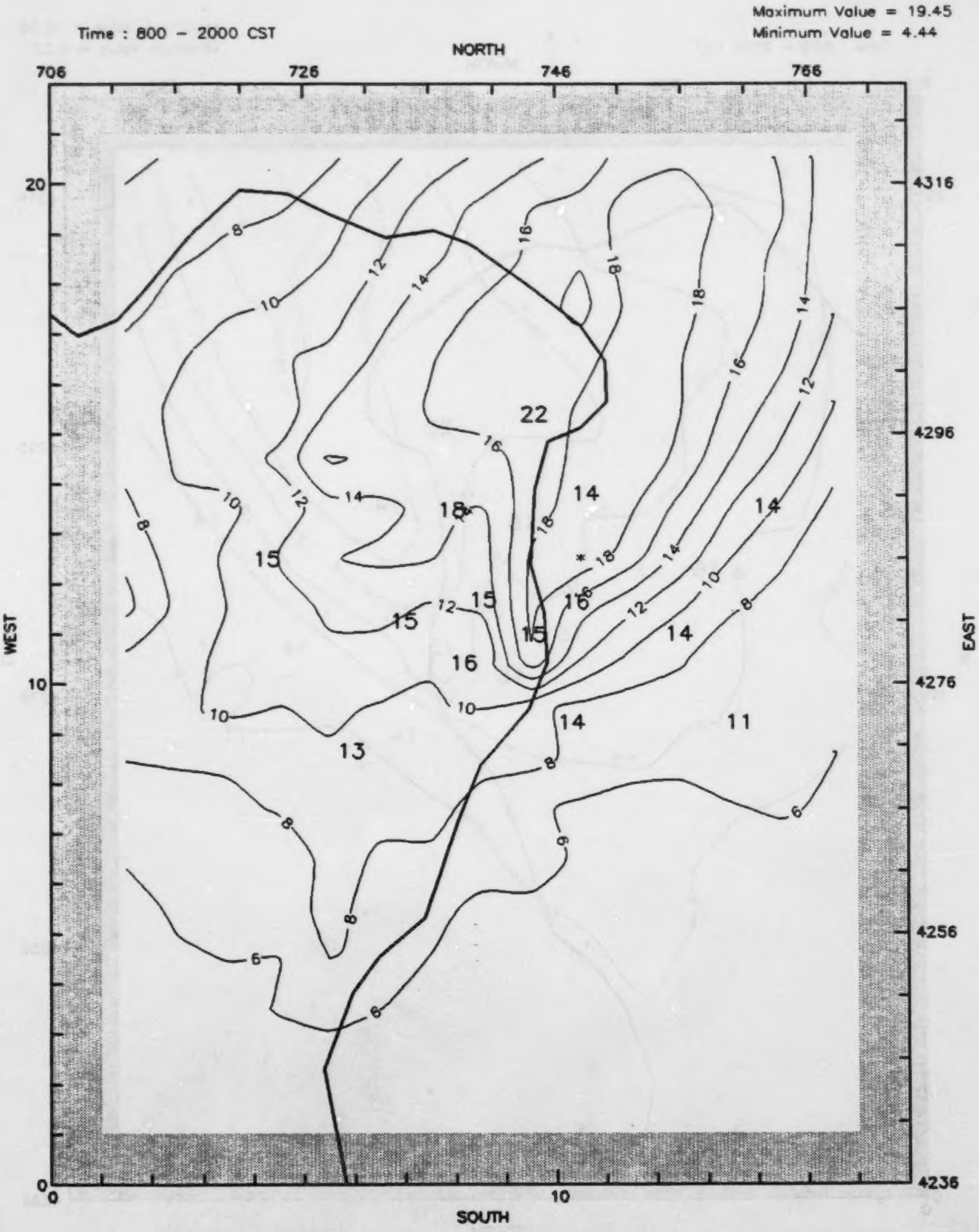
14
16

FIGURE 3-6. Isopleths of predicted maximum daily ozone concentrations (pphm) with superimposed maximum daily observations for PLANR diagnostic run #2.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Maximum Value = 19.45
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726
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766
20
10
0
0
10
4316
4296
4276
4256
4236
22
18
15
15
15
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16
16
14
14
14
14
11
13
8
10
12
14
16
18
6

FIGURE 3-7. Isopleths of predicted maximum daily ozone concentrations (pphm) with superimposed maximum daily observations for PLANR diagnostic run #3 (PLANR UAM).

the observations indicate the highest ozone concentrations should be slightly north of the center of the modeling domain. The lack of any observations in the northeastern portion of the modeling region does not discount the possibility that elevated ozone concentrations existed in that region. However, diagnostic run 3 does a much better job of placing the predicted cloud of elevated ozone concentrations in the upper center of the modeling domain (see Figure 3-7).

The predicted region-wide maximum (19.5 pphm) is within 12 percent of the observed peak (22.2 pphm) and is located approximately 11 km south-southeast from the observed peak ozone. At the location of the observed peak, run 3 predicts a daily maximum concentration of 16.7 pphm, about 25 percent of the observed value. Model performance for run 3 is remarkably better than for runs 1 and 2. Run 3 satisfies the two model performance goals and the predicted peak ozone is located well within the interior of the region. Thus run 3 is deemed an acceptable base case.

Figure 3-8 compares the predicted and observed ozone concentrations at each monitoring site for all three runs. The results from run 3 are in better agreement with the observations than are the other runs except for sites 108, where run 2 is better, and site 116, where run 1 is better. The performance of the UAM in the base case for the PLANR application to St. Louis (diagnostic run 3) is discussed further in the next section.

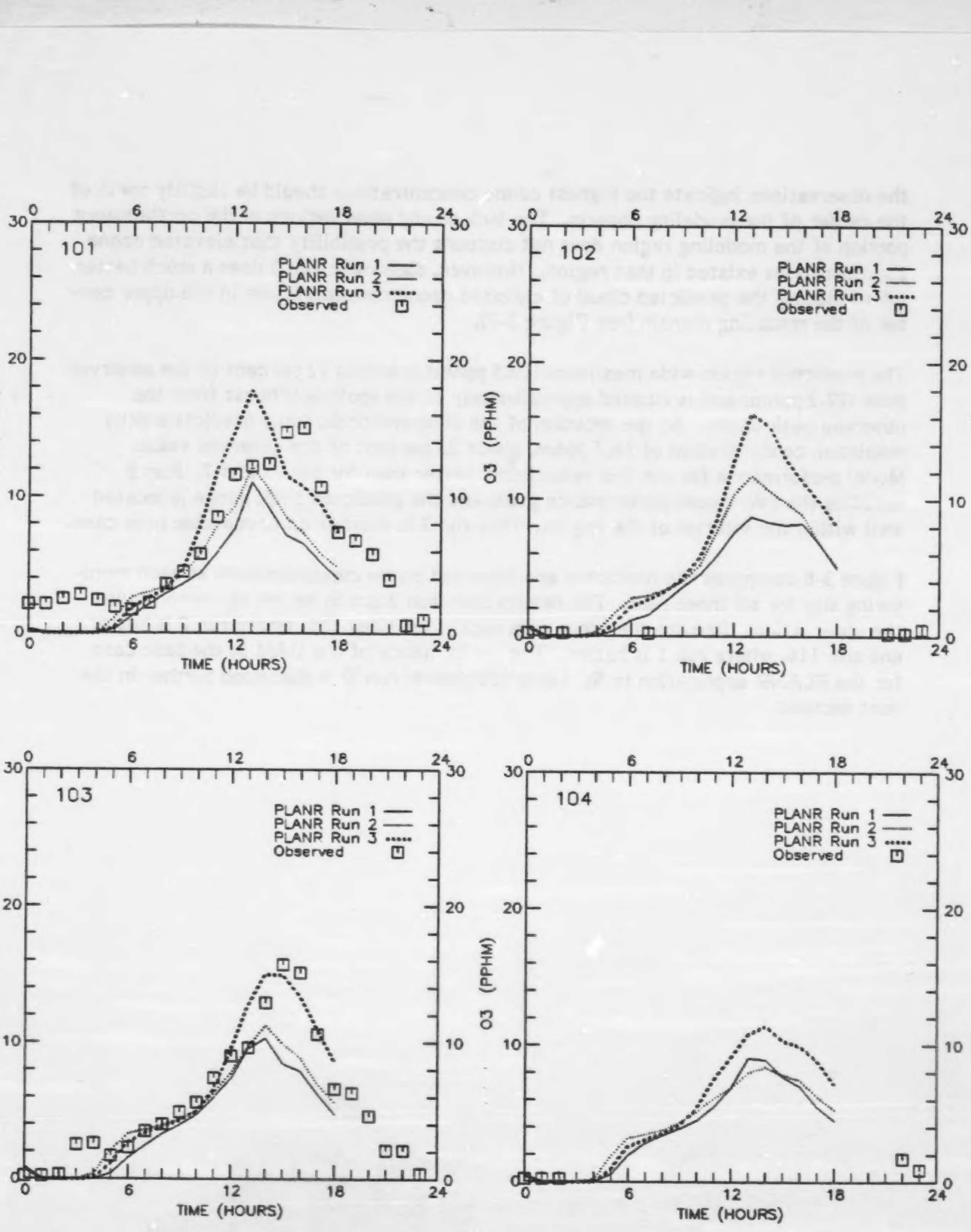


FIGURE 3-8. Comparison of hourly predicted and observed ozone concentrations at each ozone monitoring site for PLANR diagnostic runs 1, 2, and 3.

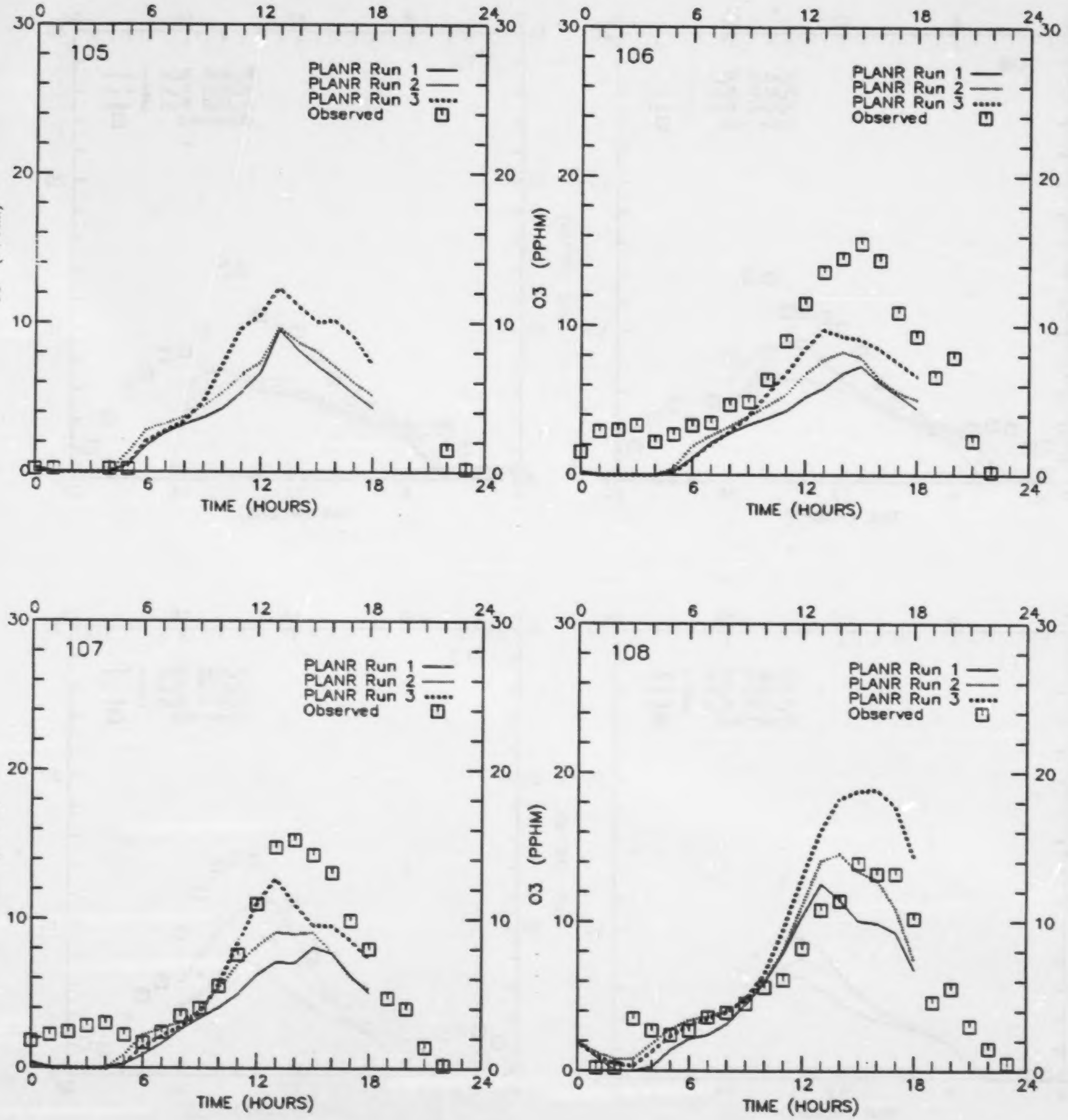


FIGURE 3-8 Continued.

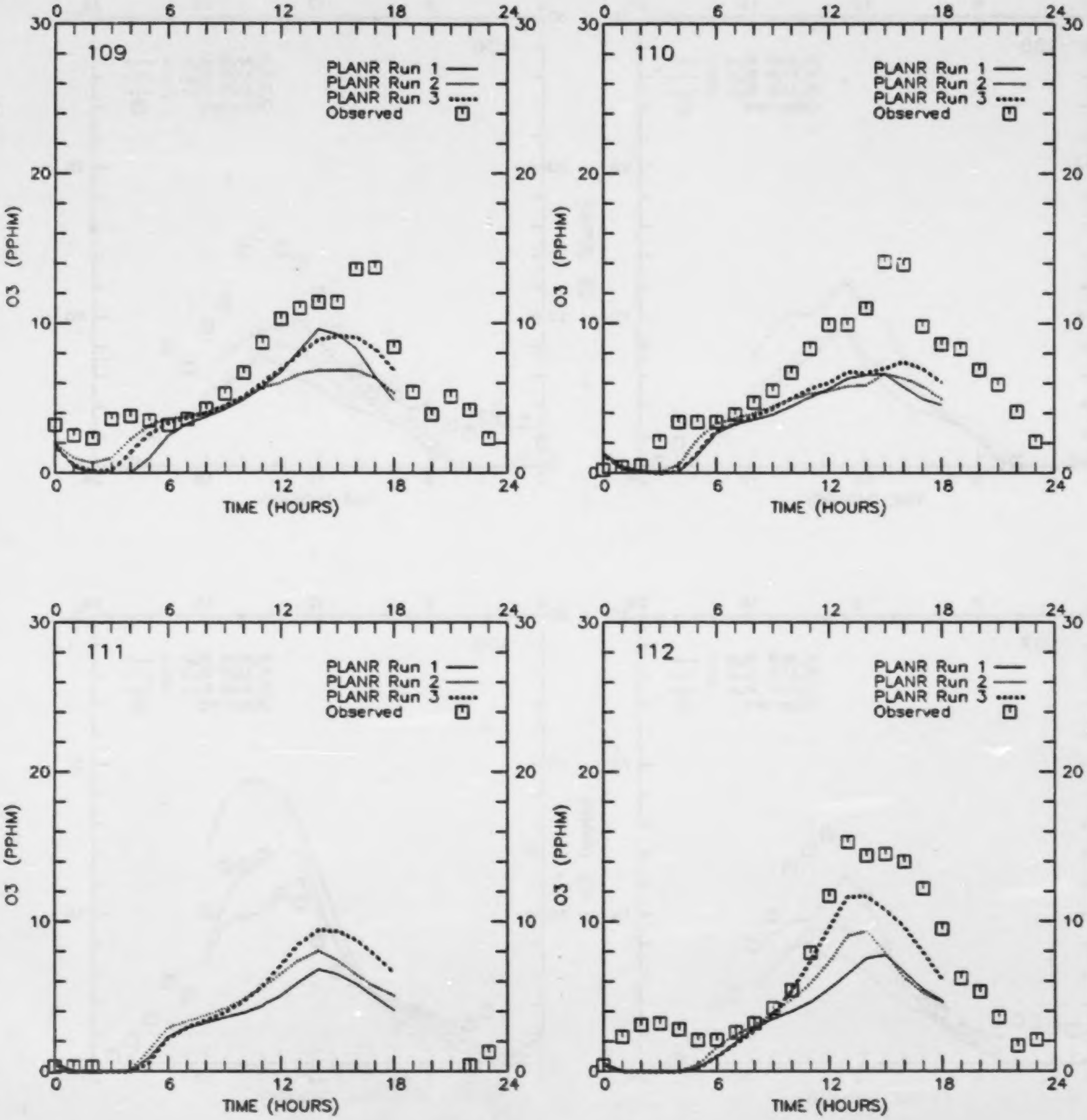


FIGURE 3-8 Continued.

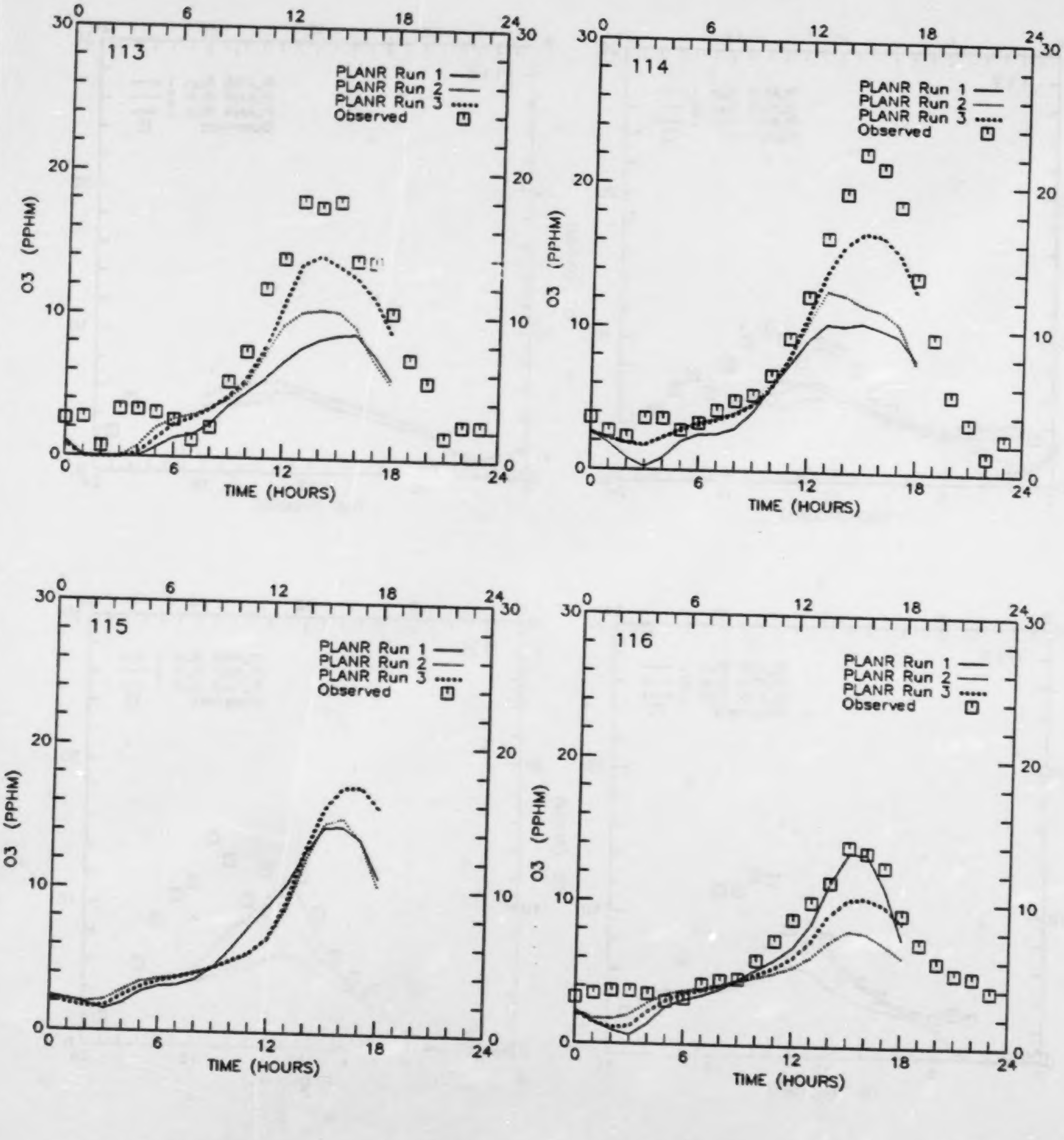


FIGURE 3-8 Continued.

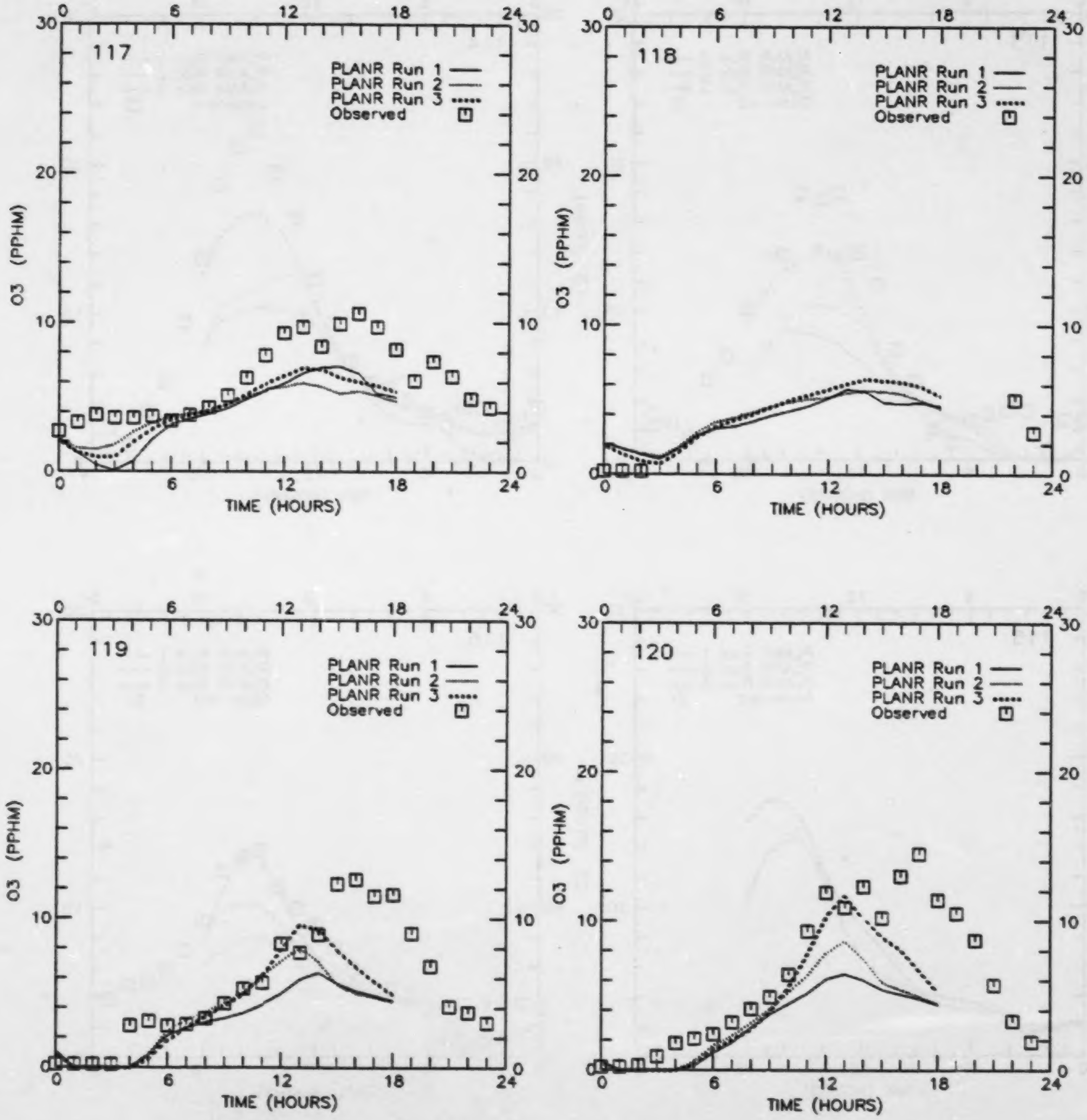


FIGURE 3-8 Continued.

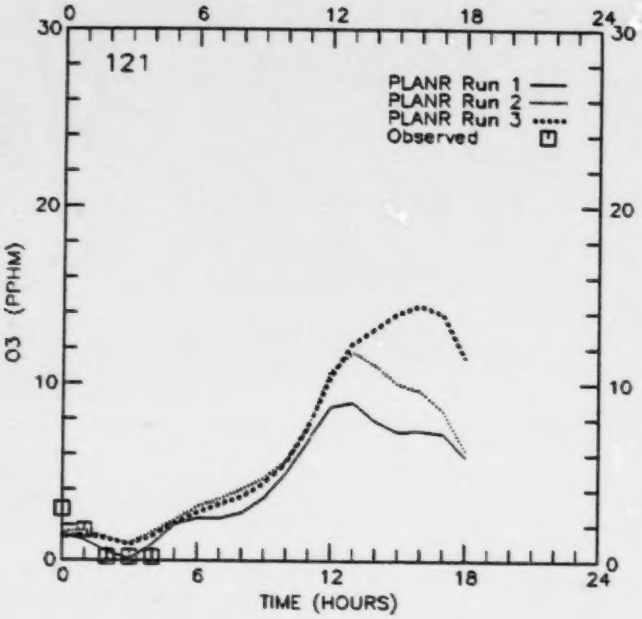


FIGURE 3-8 Concluded.

4 EVALUATION OF THE PLANR UAM APPLICATION TO ST. LOUIS

In this section we evaluate the PLANR UAM application to St. Louis by comparing the model performance of UAM when four types of input data are used: RAPS, PLANR, SIMPLE UAM(CB-IV), and UAM(CB-II); and then compare how ozone concentrations calculated by the RAPS, PLANR, and SIMPLE UAM respond to emission control scenarios. The purpose of this intercomparison is twofold: (1) to determine whether the use of only routinely available data (PLANR UAM) produces acceptable model performance; (2) to determine the minimum input data needed to obtain adequate UAM performance; to determine how model performance effects emission control strategies designed to show attainment of the ozone NAAQS; and to analyze different procedures for using the UAM to show attainment.

MODEL INPUTS

Historical UAM(CB-II)

Inputs for the UAM(CB-II) were prepared from the RAPS intensive measurement data using and the old UAM preprocessor programs (Schere and Shreffler, 1982; Cole et al., 1983; Ames et al., 1985a,b). The RAPS data base included surface wind measurements at over 20 sites (see Figure 3-4) and hourly upper-air measurements at up to three sites within the city of St. Louis. The maximum afternoon mixing height was approximately 1,500 m agl. Initial concentrations and boundary conditions were interpolated from the dense air quality measurement network. Although the same intensive data base (RAPS) was used to prepare inputs for both the UAM(CB-II) and RAPS UAM, there still are slight differences in the meteorological inputs (e.g., wind fields) because different preprocessors were used.

RAPS UAM

The inputs for the RAPS UAM were based on the RAPS data base. The procedures for creating the model inputs generally followed the procedures for the PLANR application (see Section 3) except the RAPS dense surface measurement network and the RAPS hourly upper-air soundings within St. Louis were used for the wind fields and mixing heights. The maximum afternoon mixing height was approximately 1,500 m agl. Initial concentrations and boundary conditions were interpolated from the dense air quality network.

SIMPLE UAM

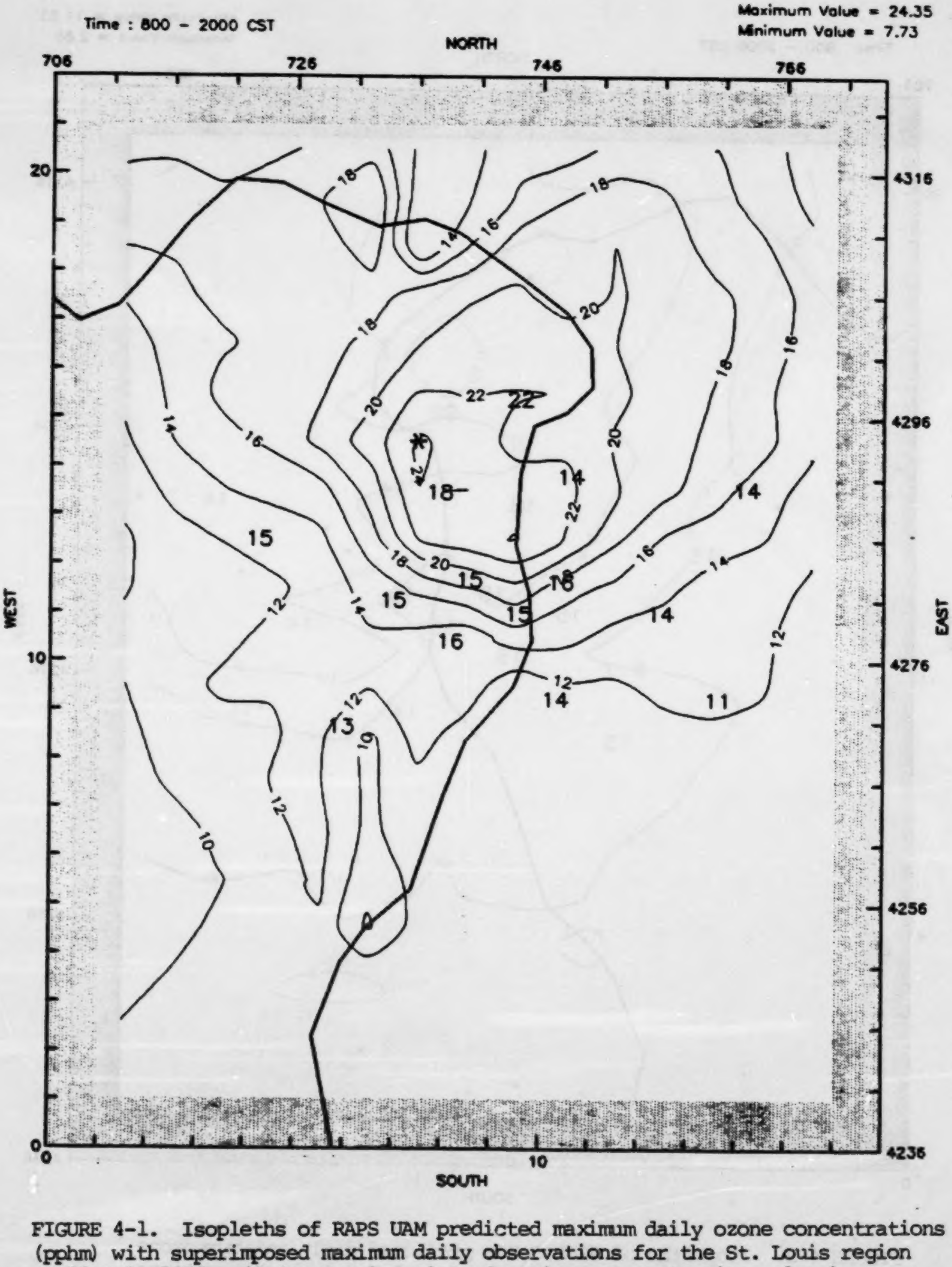
Meteorological data for St. Louis on 13 July 1976 were preprocessed by RAMMET (CRSTER) and turned into UAM wind files by assuming that the single hourly surface wind direction represented wind directions aloft and wind speeds increased with height following the stability-dependent power law wind profile. The mixing heights were assumed to be spatially constant but varied hourly. The maximum afternoon mixing height (from Salem, IL) was 2,250 m agl. The same "clean" concentration values used in the PLANR UAM were used for initial and boundary conditions.

COMPARISON OF PERFORMANCE

We compared the performance of the UAM(CB-II) and the RAPS, PLANR, and SIMPLE applications of UAM to St. Louis. Isopleths of predicted and observed daily maximum ozone concentrations from the RAPS and SIMPLE UAM applications are shown in Figures 4-1 and 4-2 (isopleths for the PLANR application are shown in Figure 3-7). Table 4-1 presents model performance statistics for the four applications. (Scatterplots and additional residual analysis plots of model performance statistics for the RAPS, PLANR, and SIMPLE applications are given in Appendix A.) Figure 4-3 shows time series plots of predicted and observed ozone concentrations at each monitoring site for the RAPS, PLANR, and SIMPLE applications.

As seen in Table 4-1 and Appendix A, calculated and observed values are very close for the RAPS simulation. The predicted region-wide maximum (24.2 pphm) overstates the observed maximum (22.2) by 9 percent and occurs approximately 9 km southwest of the observation. The predicted maximum at the location of the peak observation (21.9 pphm) is within 2 percent and occurs 2 hours later than the observed value. The RAPS UAM overpredicts the hourly ozone observations for all hours of the simulation by 10 percent and overpredicts the average of the daily maximum observations at all sites by 7 percent. The RAPS UAM with CB-IV chemistry generally produced better agreement with observations than did the RAPS UAM with CB-II chemistry.

When only routine data are used for model inputs, model performance is somewhat degraded. The PLANR UAM predicts the hourly and daily maximum observations to within approximately 20 percent on average. The predicted region-wide maximum ozone concentration (19.5 pphm) is within 12 percent of the observed maximum and occurs approximately 12 km south-southeast of the observation. The predicted maximum ozone at the location of the peak observation is within 25 percent of the observed peak ozone and occurs at the same hour as the observed peak.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4316
4296
4276
4256
4236
0
10
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22
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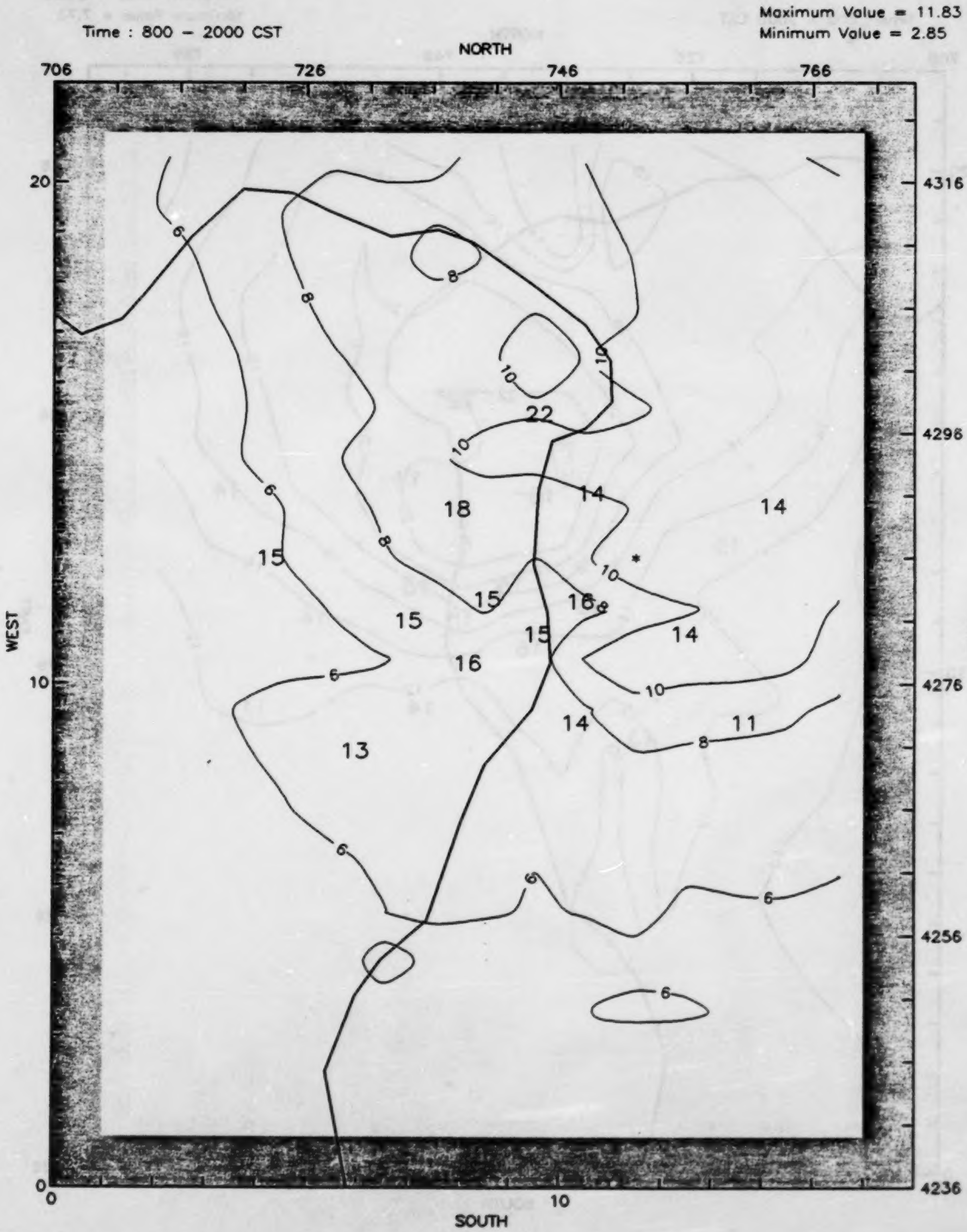
FIGURE 4-1. Isopleths of RAPS UAM predicted maximum daily ozone concentrations (pphm) with superimposed maximum daily observations for the St. Louis region on 13 July 1976. (* denotes location of maximum concentration value.)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746
766
SOUTH
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WEST
20
10
0
EAST
4316
4296
4276
4256
4236
6
8
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22
18
14
15
16
13
11

FIGURE 4-2. Isopleths of SIMPLE UAM predicted daily maximum ozone concentrations (pphm) with superimposed daily maximum observations for the St. Louis region on 13 July 1976.

TABLE 4-1. Comparison of performance statistics for four modes of application of the UAM to St. Louis for 13 July 1976.

Performance Measure	UAM (CB-II)	RAPS UAM	PLANR UAM	SIMPLE UAM
Hourly Ozone Concentrations (matched by time and location)				
Number of pairs	184*	265	265	265
Average observed (pphm)	8.3	6.8	6.8	6.8
Average predicted (pphm)	7.4	7.5	5.4	4.3
Bias (pphm)	0.9	-0.7	1.4	2.5
Average percent difference	11%	10%	21%	37%
Average absolute (gross) error	N/A	1.7	2.02	2.9
Gross error percent difference	N/A	25%	30%	43%
Correlation coefficient	0.95	0.91	0.90	0.79
Daily Maximum Ozone Concentration (matched by location but not time)				
Number of pairs	N/A	14	14	14
Average observed (pphm)	N/A	15.0	15.0	15.0
Average predicted (pphm)	N/A	16.0	12.3	8.2
Bias (pphm)	N/A	-1.0	2.7	6.8
Average percent difference	N/A	7%	18%	45%
Average absolute (gross) error	N/A	2.4	3.9	6.8
Gross error percent difference	N/A	16%	26%	45%
Correlation coefficient	N/A	0.68	0.55	0.20
Peak Ozone Concentration				
Peak observed (pphm)	22.2	22.2	22.2	22.2
Unmatched by time or location:				
Predicted region-wide maximum (pphm)	17.4	24.2	19.5	11.8
Ratio of prediction to observation	0.78	1.09	0.88	0.53
Matched by location but not time:				
Predicted maximum (pphm)	16.8	21.9	16.7	10.0
Ratio of prediction to observation	0.76	0.99	0.75	0.45
Hours difference in prediction to observation	N/A	+2	0	-2

* Due to differences in sample sizes between the historical UAM(CB-II) and the current UAM performance statistics, statistics for non-peak ozone results cannot be directly compared.

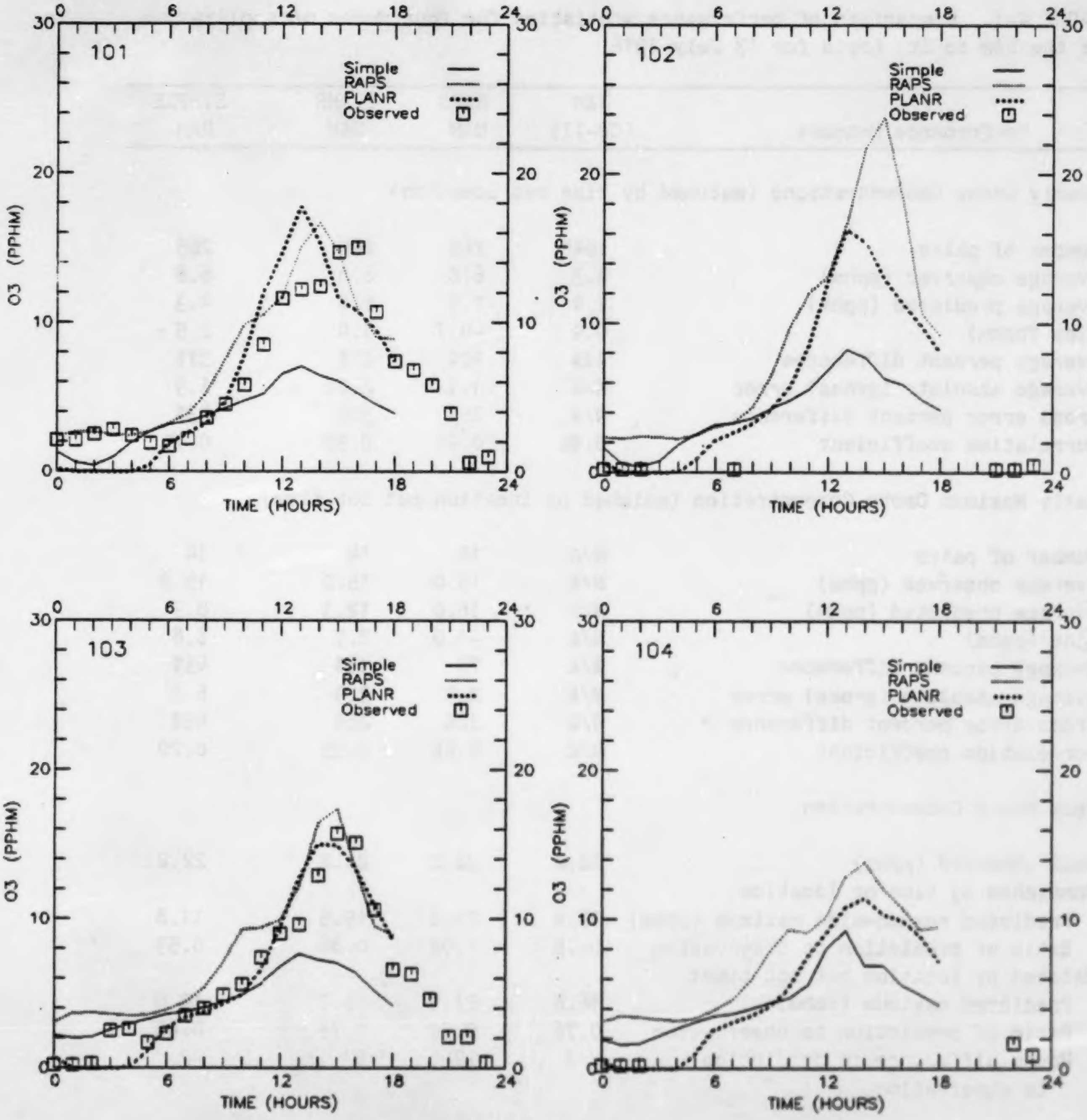

FIGURE 4-3. Comparison of predicted and observed hourly ozone concentrations (pphm) at each monitoring site for the RAPS, PLANR, and SIMPLE UAM.

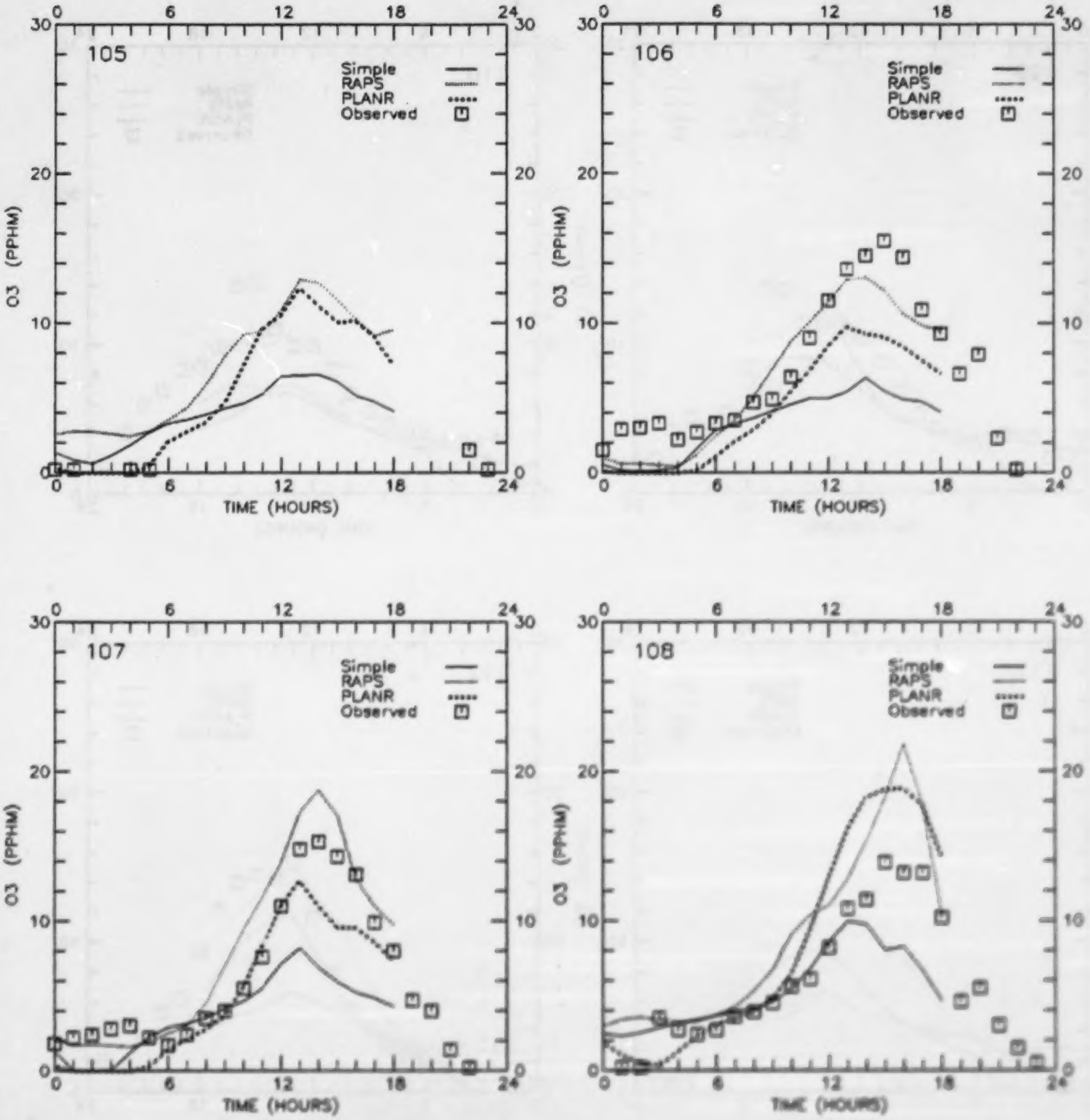

FIGURE 4-3 Continued.

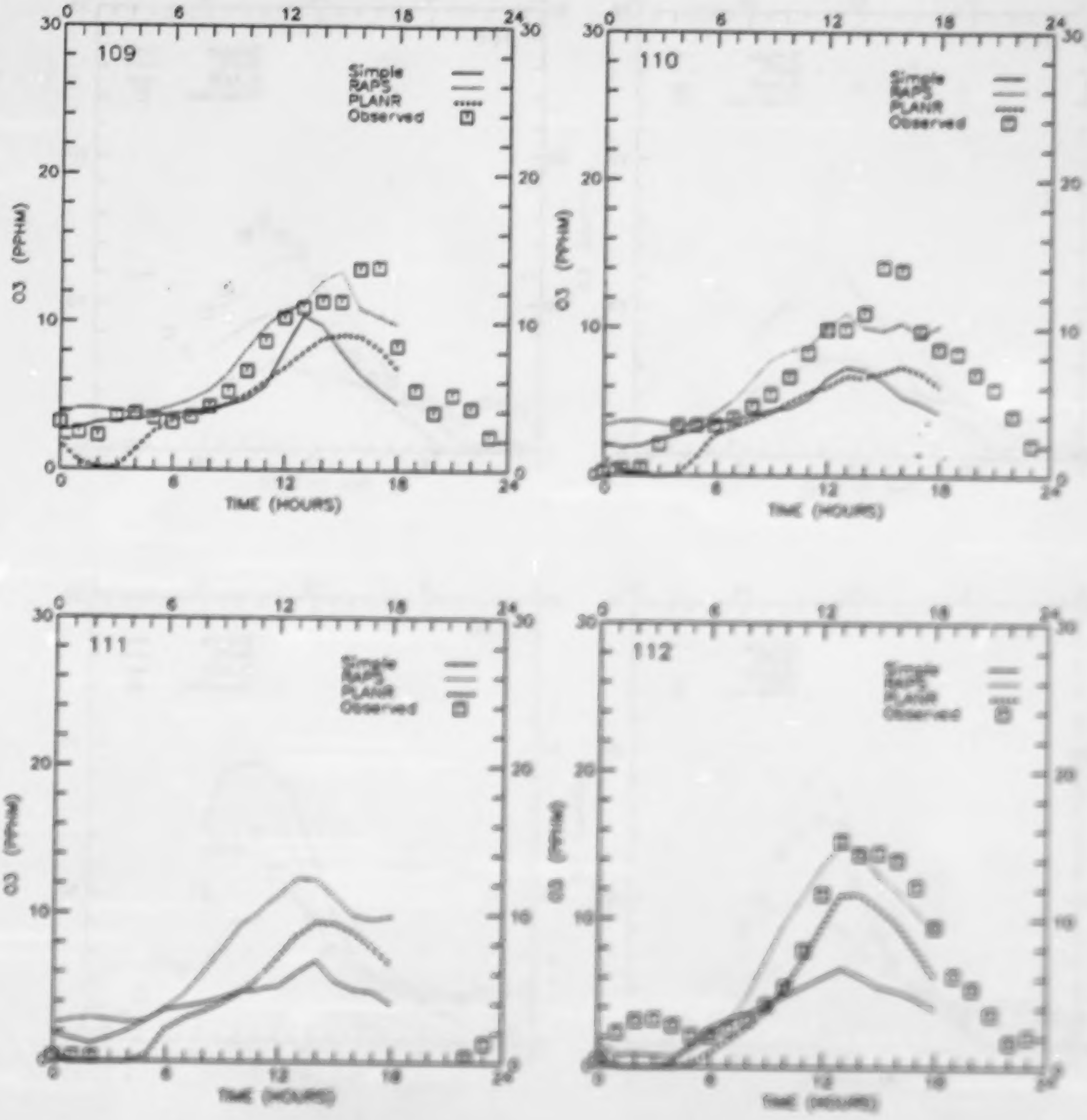

FIGURE 4-3 Continued.

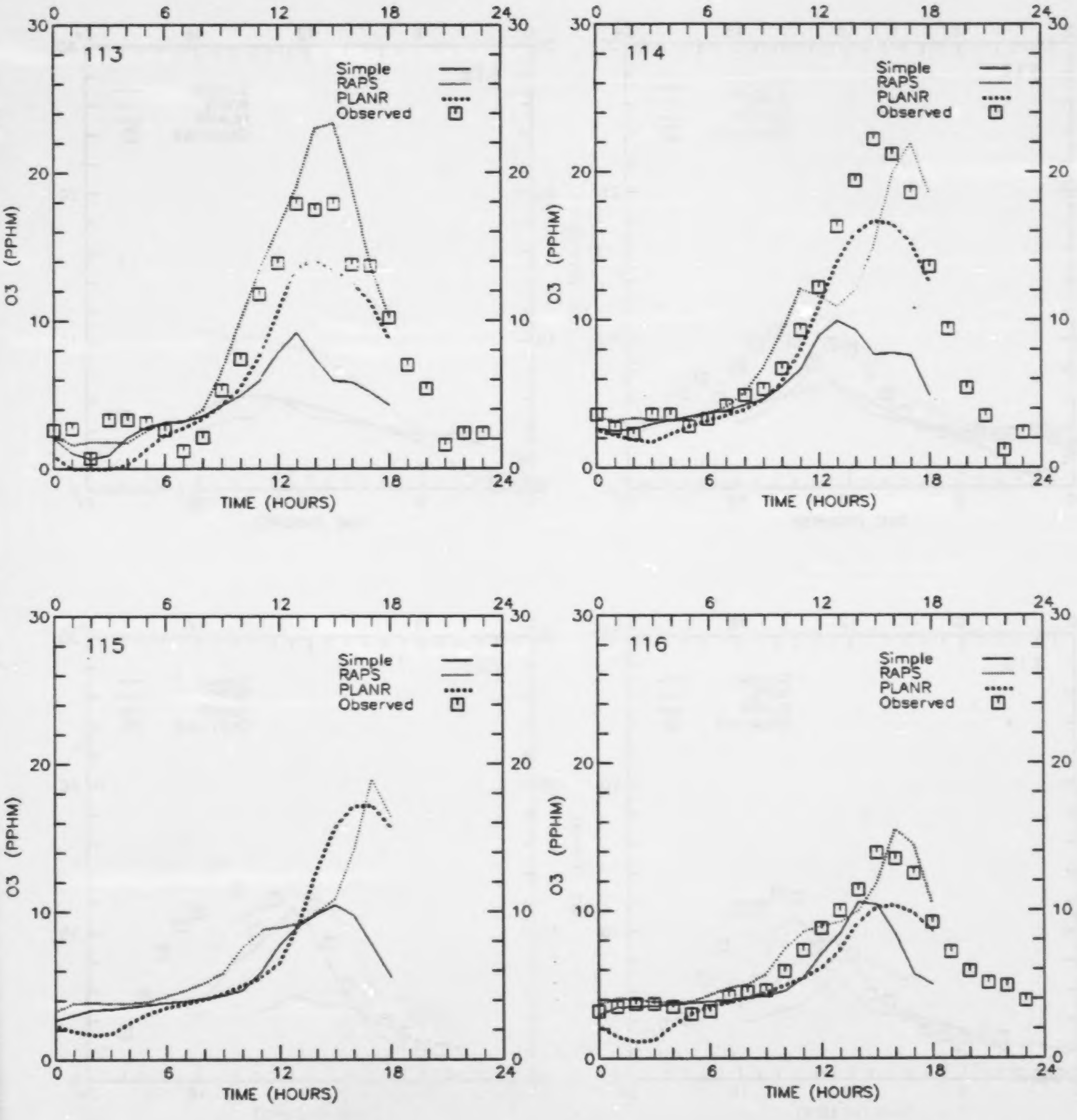

FIGURE 4-3 Continued.

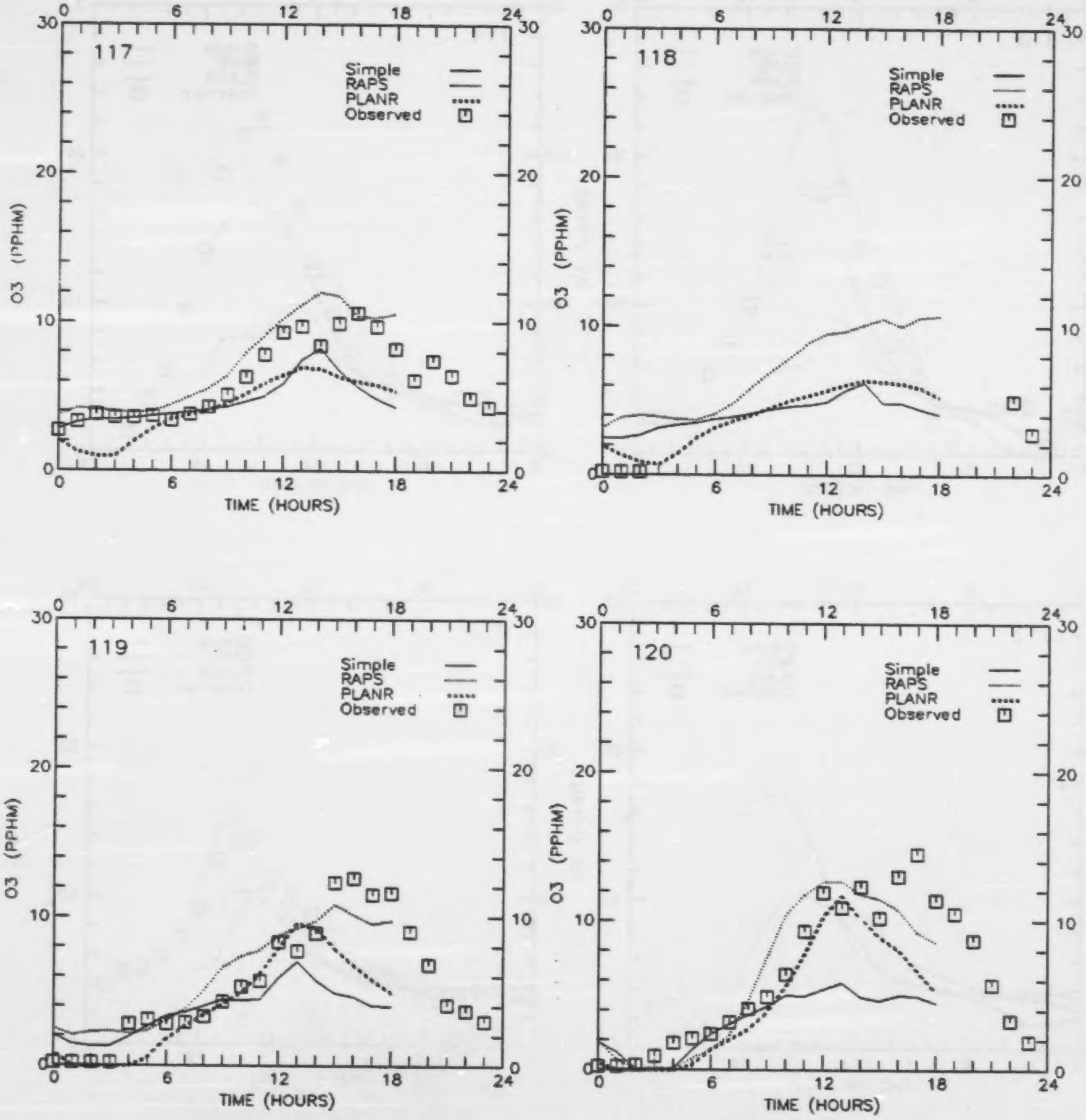

FIGURE 4-3 Continued.

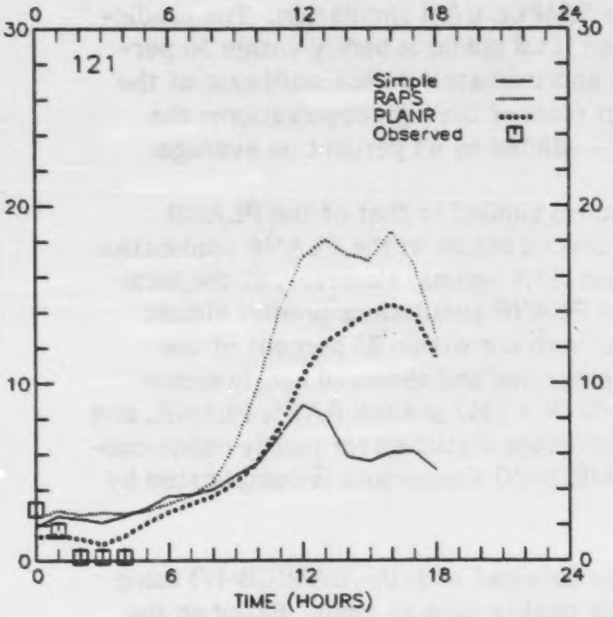

FIGURE 4-3 Concluded.

Model performance is further degraded in the SIMPLE UAM simulation. The predicted region-wide maximum ozone concentration (11.8 pphm) is barely within 50 percent of the maximum observation and occurs approximately 14 km southeast of the observation. The model tends to underpredict most of the high observations; the daily maximum ozone observations are underpredicted by 45 percent on average.

The performance of the UAM(CB-II) simulation is similar to that of the PLANR UAM. The observed peak (22.2 pphm) is reproduced better in the PLANR application (19.5 pphm) than in the UAM(CB-II) application (17.4 pphm). However, at the location of the observed peak the UAM(CB-II) and PLANR simulations predict almost exactly the same daily maximum ozone value; both are within 25 percent of the observation. Note that the sample sizes for predicted and observed hourly ozone concentrations are different in the UAM(CB-II) (N = 184) and the RAPS, PLANR, and SIMPLE UAM (N = 265). Comparison of performance statistics for hourly ozone concentrations between the UAM(CB-II) and UAM(CB-IV) simulations is complicated by this difference.

In summary, adequate model performance was obtained with the UAM(CB-IV) using only routinely available meteorological and air quality data as input. Based on the peak ozone performance measures, the PLANR performance statisfied the model performance goals and produced results that were more accurate that those obtained with the historical UAM(CB-II), which used intensively measured data. However, the PLANR use of the UAM should be evaluated for different cities before definitive conclusions can be drawn concerning the use of the UAM with limited data.

DISCUSSION

Differences in model performance between the RAPS, PLANR, and SIMPLE applications of UAM (CB-IV) and the UAM(CB-II) can be attributed primarily to differences in meteorology (winds and mixing heights), initial and boundary conditions, and, in the case of the UAM(CB-II), chemistry. The PLANR UAM predicts a lower peak ozone than the RAPS UAM, primarily because the RAPS UAM uses higher boundary conditions, but also because PLANR UAM uses higher mixing heights and wind speeds (i.e., more dilution). Even though the UAM(CB-II) also used the higher boundary conditions, the chemical mechanism (CB-II) is less reactive than the one used in the PLANR UAM application (CB-IV), which might explain why the PLANR UAM predicts a higher peak than the UAM(CB-II). The SIMPLE UAM predicts the lowest peak because it has low boundary conditions (same as PLANR UAM) and the highest mixing height and wind speeds.

The emission inputs were based on the 1976 NEDS emissions data converted to UAM(CB-II) formats as part of the St. Louis Ozone Study. In the UAM(CB-IV) simulations (RAPS, PLANR, and SIMPLE) the chemical speciation of the emissions may be improperly characterized since the VOC emissions in CB-IV were estimated from their CB-II counterparts rather than from the original compositions of individual species. It is unclear whether such improper characterization results in an over- or underestimate of the emissions reactivity in the UAM(CB-IV) simulations.

Since the development of the 1976 emission inventory for UAM modeling, many new VOC emissions sources have been recognized. These emissions include natural emissions, motor vehicle running loss emissions, and previously unaccounted evaporative sources, such as solvents, paints, and coatings. The underprediction of the observed peak ozone concentrations by the PLANR UAM and UAM(CB-II) could be due entirely to the absence of these emissions. Conversely, the seemingly good agreement between observed ozone concentrations and concentrations predicted by the RAPS UAM may be because other UAM inputs were incorrectly specified, thus offsetting the understatement of the emission inventory. The most likely UAM inputs in the RAPS UAM that may be offsetting the understatement of the emissions include overestimates of the initial and boundary conditions and overestimates of the reactivity of the emissions.

The RAPS UAM initial and boundary conditions were based on the dense surface air quality network from the RAPS data base, whereas the PLANR and SIMPLE UAM used "clean" values (25 ppbc VOC and 1 ppb NO_x). The use of surface air quality data to characterize concentrations aloft invariably results in overestimates of the initial pollutant mass and the pollutant mass flux entering the region. If the initial or boundary concentrations in the RAPS UAM are overspecified, then the model will estimate higher emission control requirements to meet attainment than are actually needed. Since the RAPS UAM does not tend to systematically overpredict the observed concentrations at ozone sites upwind of the urban core (see Figure 4-3), it is more likely that the RAPS initial concentrations have been overstated.

This discussion is speculative at best, but it does illustrate that good model performance does not always indicate that the model is operating correctly. Because of the underestimation of emissions in the 1976 emission inventory we would expect the UAM to underpredict the peak observed ozone concentration. Thus the seemingly good performance of the RAPS UAM is questionable. This exercise does illustrate two important points. First, adequate UAM model performance evaluation is a necessary but not a sufficient condition for defining a proper UAM base case. An evaluation of whether the model is getting the right answer for the right reason is also necessary. Second, an accurate emissions inventory is essential for using any photochemical model to calculate emissions control strategies to demonstrate attainment of the ozone NAAQS.

CORRECTIONS FOR MODEL BIAS IN CALCULATIONS OF OZONE REDUCTIONS IN RESPONSE TO EMISSION CONTROL STRATEGIES

Although the performance of the PLANR UAM application to St. Louis is adequate using just routine data, it is unclear at this time how the UAM will be used to evaluate alternative emission control strategies when the observed ozone peak is not well replicated. Model bias (either over- or underprediction of the observed peak) needs to be accounted for when using a model to demonstrate attainment of the ozone NAAQS. This report is not the forum to propose a policy for the use of the UAM to demonstrate NAAQS attainment. However, the recent development of several sets of UAM inputs (RAPS, PLANR, and SIMPLE UAM) allows us to compare several methodologies for accounting for model bias and what effects data availability will have on the calculated emission reduction requirements.

When using just routine data and a limited number of diagnostic simulations (PLANR UAM) we cannot expect to replicate the peak ozone observations, thus some measure of accounting for the model bias needs to be incorporated into the PLANR procedures for demonstrating ozone attainment.

We have initially identified three methodologies for using the UAM to demonstrate attainment of the ozone standard, two of which will correct for model bias:

(1) Uncorrected bias approach. The model predictions are used as they are. That is, regardless of the difference between the observed peak and the predicted region-wide maximum in the base case, an emission control scenario is considered to demonstrate attainment of the ozone NAAQS when the predicted region-wide maximum in response to emission reductions is reduced to the NAAQS level (12 pphm).

In the next two methods the difference between the predicted region-wide maximum ozone concentrations in the base case and in an emission reduction scenario is compared with the difference between the observed peak and the ozone NAAQS.

(2) The decrement approach. The emission reduction needed to reduce the predicted regional maximum ozone to the NAAQS level is the same incremental reduction as that needed to reduce the observed peak. For example, if the observed and predicted peaks are respectively 22 and 20 pphm, an emission control strategy demonstrates attainment of the ozone NAAQS when the predicted region-wide maximum is reduced by 10 pphm (i.e., the increment from the observed peak of 22 pphm to the ozone NAAQS, 12 pphm).

(3) The percentage adjustment approach. The emission reduction needed to reduce the predicted peak ozone is the same percentage reduction needed to reduce the observed peak. For the example of observed and predicted peaks of 22 and 20 pphm, an emission control scenario demonstrates attainment when it reduces the predicted region-wide maximum by 45 percent, i.e., to 10.9 pphm, the same percentage required to reduce the observed peak to 12.0 pphm.

Variants of these approaches include taking into account an irreducible amount of background ozone, which is unaffected by anthropogenic emission reductions, and using the maximum predicted ozone concentration at the location of the observed peak instead of the region-wide predicted maximum ozone. In the following sections we demonstrate how each of these approaches would work for the RAPS, PLANR, and SIMPLE UAM applications with across-the-board VOC emission reductions.

For this illustrative example we have neglected any effects of emission changes to NO_x, which will greatly effect the control strategies.

Three VOC emission scenarios were simulated by the RAPS, PLANR, and SIMPLE UAM: the base case and a 60 percent and 80 percent reduction in VOC emissions. Table 4-2 shows the predicted region-wide maximum ozone concentrations for the different emission scenarios. In the following sections we discuss how to estimate the VOC emission reduction required to reduce the observed peak ozone to 0.12 ppm using the methodologies discussed above.

Uncorrected Bias

Figure 4-4 shows the predicted peak ozone reductions for different VOC emission reduction scenarios as calculated in the RAPS, PLANR, and SIMPLE UAM applications. If the model predictions were used as is, the SIMPLE UAM estimates that no emission reduction is required to reduce the peak ozone concentrations to 12 pphm because of its gross underprediction of the observed peak. The PLANR UAM estimates that a 55 percent VOC emission reduction is required, and the RAPS UAM estimates that a 91 percent VOC emission reduction is required.

The difficulty in interpreting the modeling results is complicated by the fact that a region is considered in nonattainment of the ozone NAAQS when the fourth highest measured daily maximum ozone concentration in three years for a region exceeds 12.4 pphm. The RAPS UAM does a very good job of predicting the peak observed ozone concentration at the location of the observed peak (within 2 percent) but it predicts a higher region-wide maximum than the peak observation. It is impossible to determine whether such a higher ozone concentration actually existed in St. Louis on 13 July 1976 because no ozone monitors existed at the location of the predicted peak.

The EPA recommends that emission control requirements should not be based on ozone predictions constrained to a particular monitoring site (Layland and Cole, 1983). However, if the RAPS UAM predicted region-wide maximum ozone concentration is an overprediction of actual ozone concentrations for this day, then the calculated VOC emission reductions needed to eliminate exceedances of the ozone NAAQS may be overstated. If VOC emission reductions are based on the ozone concentration predicted by the RAPS UAM at the location of the highest observed ozone, a 78 percent reduction would be required to eliminate the ozone exceedance on this day, in contrast to the 91 percent reduction based on the region-wide maximum ozone prediction.

TABLE 4-2. Predicted regional maximum ozone concentrations for the RAPS, PLANR, and SIMPLE UAM applications for different VOC emission reduction scenarios.

Percent VOC Emission Reductions	Predicted Regional Maximum Ozone Concentration (pphm)		
	RAPS	PLANR	SIMPLE
0	24.35	19.45	11.83
60	17.73	11.80	8.91
80	14.27	8.48	7.17

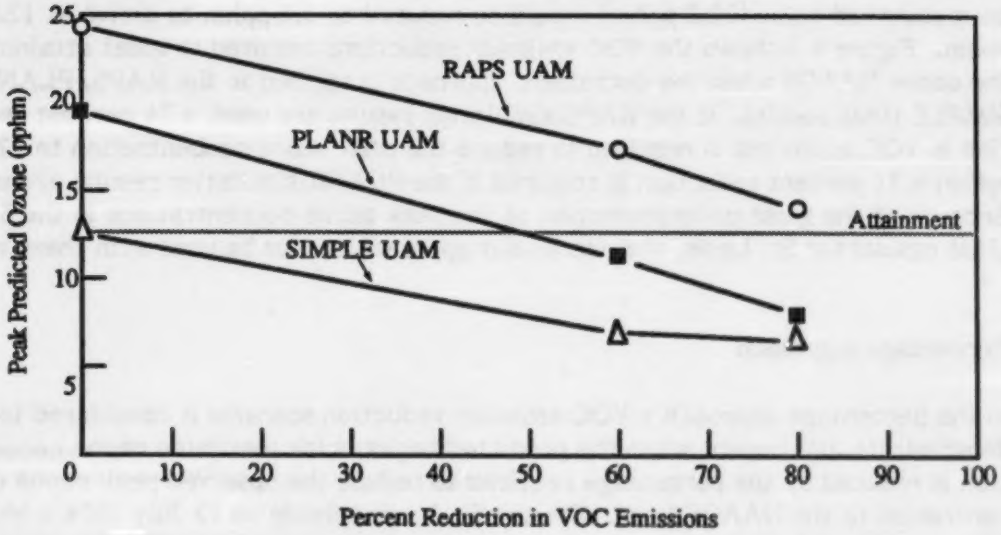

FIGURE 4-4. Region-wide maximum ozone concentrations calculated by the RAPS, PLANR, and SIMPLE UAM for three scenarios in St. Louis, 13 July 1976 (0, 60, and 80 percent reductions in VOC emissions).

Decrement Approach

In the decrement approach a VOC emission reduction scenario is considered to demonstrate attainment when the predicted region-wide maximum ozone concentration is reduced by the amount needed to reduce the peak observed ozone to the NAAQS level. For the St. Louis episode on 13 July 1976 this would mean that the peak observed value (22.2 pphm) should be reduced by 9.8 pphm to arrive at 12.4 pphm. Figure 4-5 shows the VOC emission reductions required to meet attainment of the ozone NAAQS when the decrement approach is applied to the RAPS, PLANR, and SIMPLE UAM results. If the RAPS simulation results are used, a 74 percent reduction in VOC emissions is required to reduce the peak ozone concentration to 12.4 pphm; a 71 percent reduction is required if the PLANR simulation results are used. Because of the gross underprediction of the peak ozone concentrations in the SIMPLE UAM results for St. Louis, the decrement approach cannot be used with these results.

Percentage Approach

In the percentage approach a VOC emission reduction scenario is considered to demonstrate attainment when the predicted region-wide maximum ozone concentration is reduced by the percentage required to reduce the observed peak ozone concentration to the NAAQS level. For the St. Louis episode on 13 July 1976 a 44 percent reduction in the peak ozone is required to reduce the observed ozone concentration to 12.4 pphm. Figure 4-6a shows the VOC emission reductions needed for ozone attainment when the percentage approach is applied to the RAPS, PLANR, and SIMPLE UAM results (83, 66, and 90 percent respectively).

One potential problem with the percentage approach is the failure to account for background ozone. Both the decrement and percentage methods are complicated by background ozone assumptions. As the predicted ozone approaches background levels, the sensitivity of the predicted ozone concentrations to emission controls is reduced. Thus when the model underpredicts the peak observed ozone concentration, the decrement and percentage methods will overstate.

SUMMARY

Table 4-3 summarizes the percentage VOC emission reductions required to reduce the peak observed ozone concentrations to below the ozone NAAQS for several methods using the RAPS, PLANR, and SIMPLE UAM. When model calculations are used without adjustment (uncorrected bias), the emission reduction requirements are understated if the model underpredicts the observed peak ozone (i.e., PLANR and SIMPLE UAM) and overstated when the model overpredicts the peak ozone (RAPS UAM). Thus it is appears that when the model underpredicts, the predicted ozone

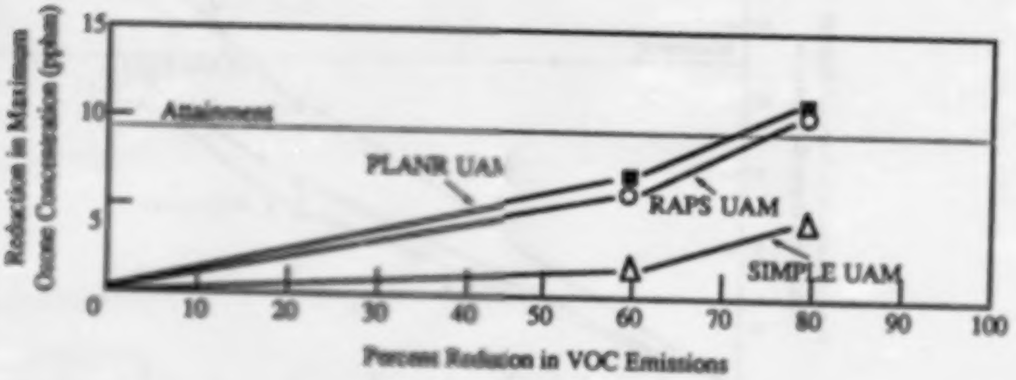

FIGURE 4-5. Use of the decrement approach to correct predicted region-wide maximum ozone concentrations tdemonstrate attainment of the NAAQS. The predictions are from the RAP, PLANR, and SIMPLE UAM applications to three scenarios in St. Louis (seeFigure 4-4). The attainment line is the reduction needed to reduce the observed peak ozone to below the NAAQS.

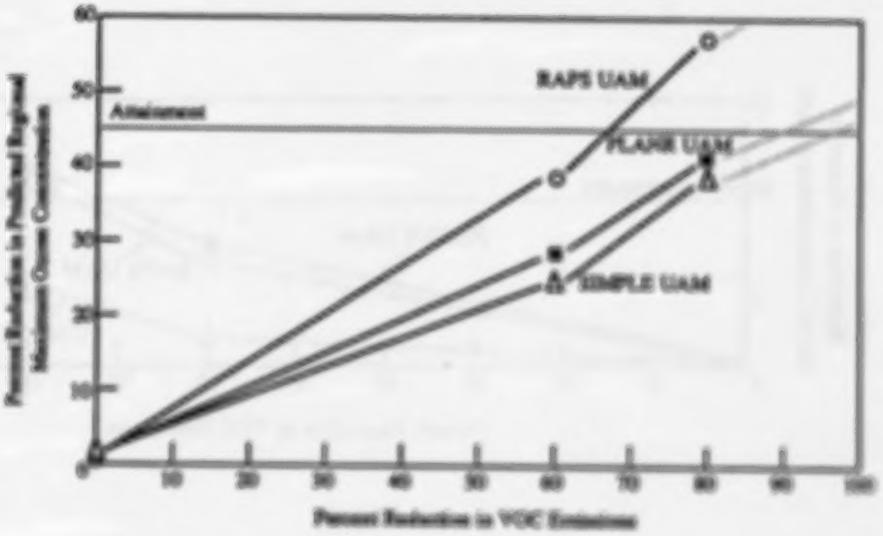

FIGURE 4-6. Use of the percentage approach to correct predicted region-wide maximum ozone concentrations to demonstrate attainment of the NAAQS. The predictions are from the RAPS, PLANR, and SIMPLE UAM applications to three scenarios in St. Louis (see Figure 4-4). The attainment line is the reduction needed to reduce the observed peak to below the NAAQS.

TABLE 4-3. Estimated reduction in VOC emissions required to meet attainment of the ozone NAAQS. Different estimation methods were applied to the RAPS, PLANR, and SIMPLE UAM results.

Method	Percent VOC Emission Reduction Requirement		
	RAPS	PLANR	SIMPLE
Uncorrected bias approach	91[a]/78[b]	55[a]	0[a]
Decrement approach	78	73	>100
Percentage approach	83	66	90
Percentage approach with background	82	64	79

[a] Using predicted region-wide ozone concentrations.

[b] Using predicted ozone concentrations at the location of the observed peak.

concentrations should not be used as is to demonstrate attainment of the ozone standard. In contrast, when the model overpredicts, the model calculations can be used as is to obtain a conservative estimate of the necessary emission reduction.

When model bias is accounted for (using the decrement or percentage method), the PLANR and RAPS UAM results produce quite similar estimates of the VOC emission reductions. The estimates vary by less than 10 percent. However, the SIMPLE UAM produces estimates that are quite variable and not consistent with each other. This is not desirable and indicates that when the UAM performs extremely poorly, as in the SIMPLE UAM, then the model should not be used to demonstrate attainment of the ozone NAAQS.

Comparison of the decrement and percentage methods of estimating VOC emission reductions reveals that, for the St. Louis episode on 13 July 1976, the RAPS UAM leads to 5 to 10 percent more reductions than does the PLANR UAM.

5 DEVELOPMENT OF A PLANR UAM BASE CASE IN PHILADELPHIA

Because we wished to compare the PLANR UAM modeling results for Philadelphia with those from certain previous studies of this region (Haney and Braverman 1985; Haney and Burton, 1988), we used the same modeling domain (Figures 5-1 and 5-2) and modeling period (0000 to 2000 on 13 July 1979) used in the earlier studies. Most of the remaining PLANR UAM modeling inputs were quite different because the PLANR UAM inputs were developed using just routine meteorological and air quality data.

METEOROLOGICAL CONDITIONS

Our characterization of meteorological conditions in Philadelphia on 13 July 1979 was based on daily weather maps, routine surface meteorological data in the region (Table 5-1), routine twice-daily upper-air observations from John F. Kennedy (JFK) International Airport (New York City) and Dulles International Airport (Washington, DC), and ozone concentrations from the routine air quality modeling network (Table 5-2). The winds on 12 and 13 July were very light due to the presence of a high-pressure system located off of the coast of Florida (i.e., a Bermuda high). As seen in the daily weather map (Figure 5-3) the high-pressure system dominated the surface and aloft wind fields. On 13 July the high-pressure system weakened during the course of the day, due to the movement of a trough that resulted from remnants of Hurricane Bob, and moved eastward into western Pennsylvania. It is postulated that the high observed ozone concentrations on 13 July were due to stagnant conditions on the 12th and the morning of the 13th.

On the afternoon and evening of 12 July surface winds were light and mainly from the west-northwest. By early morning, on 13 July most of the surface winds were calm, with some wind monitors recording very light winds from the north. The winds remained fairly light during the early morning of 13 July and then became southerly by 1000 EST. Under this flow regime it is assumed that pollutants from Phildelphia traveled a short distance south during 12 July and early morning on the 13th, and then north across the city after the wind shift at 1000. Such recirculation of the 12 July emissions on 13 July is most likely the cause of the high ozone concentrations recorded on 13 July.

The presence of high amounts of ozone and ozone precursors in Philadelphia on the morning of 13 July is also evident in the routine ozone monitoring data. Observed

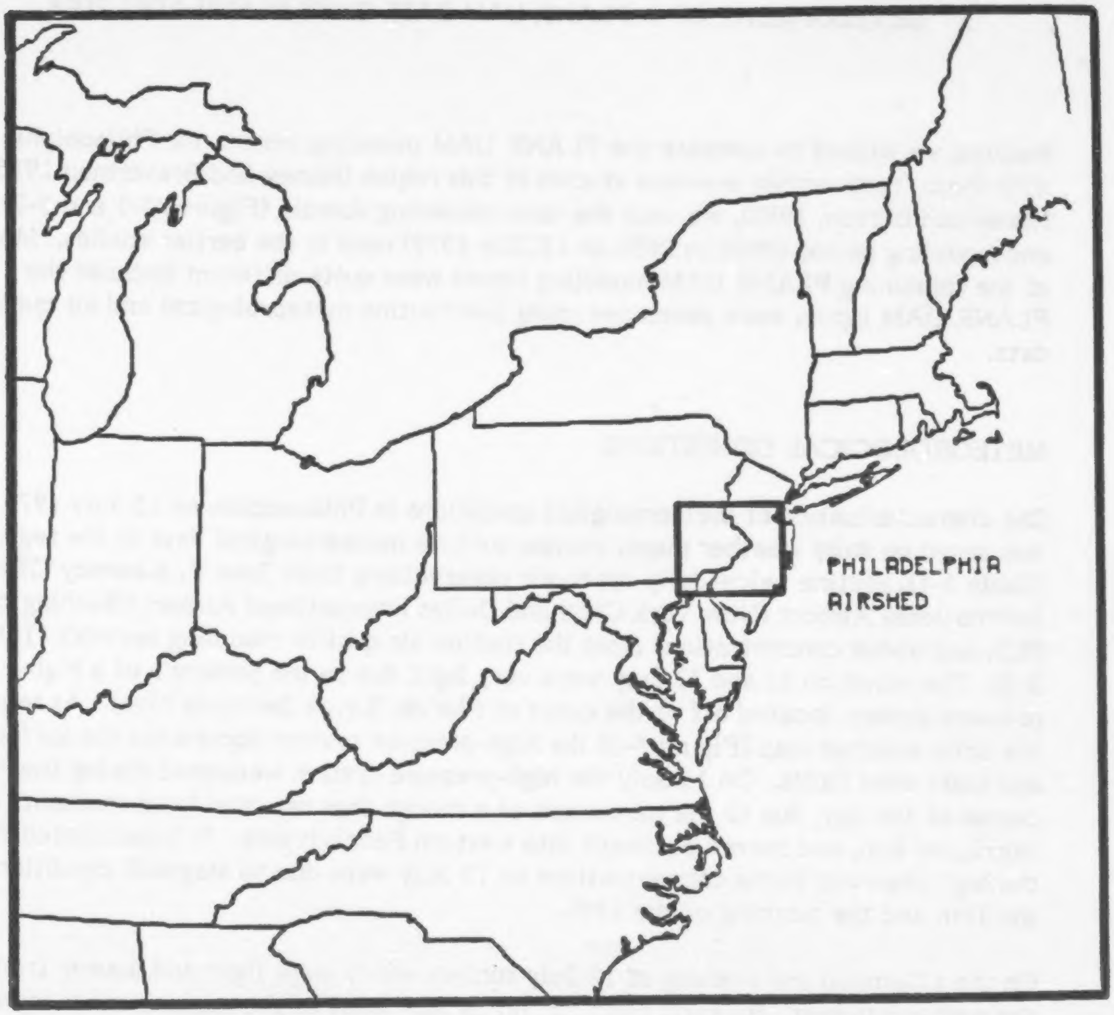
PHILADELPHIA
AIRSHED

FIGURE 5-1. Geographical location of the Philadelphia airshed modeling region. (Source: Haney and Braverman, 1985)

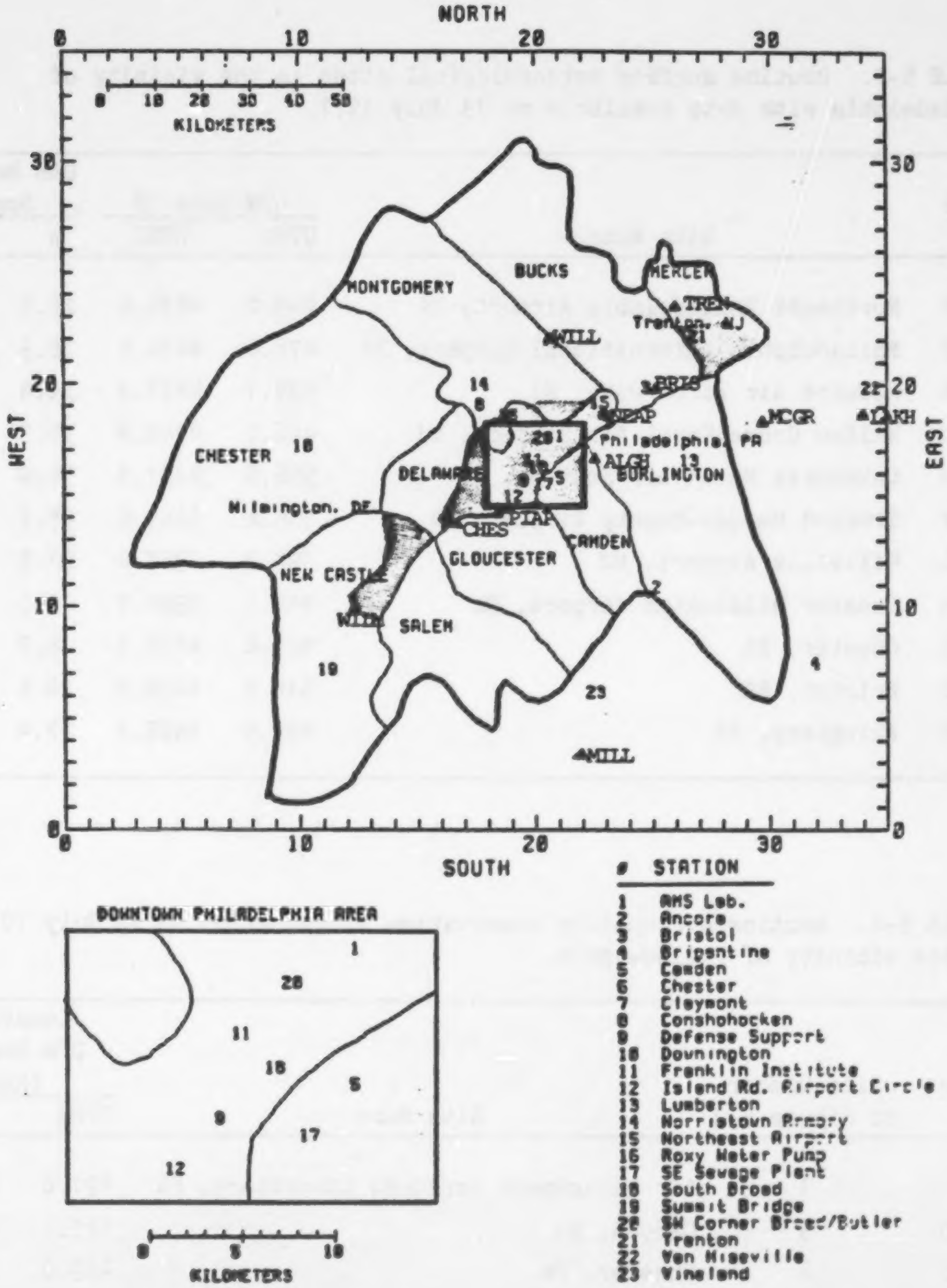
NORTH
SOUTH
WEST
EAST
0
10
20
30
KILOMETERS
MONTGOMERY
BUCKS
MERCER
TREN
Trenton, NJ
WILL
BRIS
MCGR
LAKH
CHESTER
DELAWARE
Philadelphia, PA
ALGH
BURLINGTON
NEAP
Wilmington, DE
CHES
PIAP
CAMDEN
GLOUCESTER
NEW CASTLE
WILM
SALEM
MILL
DOWNTOWN PHILADELPHIA AREA
# STATION
1 AMS Lab.
2 Ancora
3 Bristol
4 Brigantine
5 Camden
6 Chester
7 Claymont
8 Conshohocken
9 Defense Support
10 Downingtown
11 Franklin Institute
12 Island Rd. Airport Circle
13 Lumberton
14 Norristown Armory
15 Northeast Airport
16 Roxy Water Pump
17 SE Sewage Plant
18 South Broad
19 Summit Bridge
20 SW Corner Broad/Butler
21 Trenton
22 Von Hiseville
23 Vineland

FIGURE 5-2. Philadelphia airshed modeling region. Philadelphia AQCR for which emissions are available is shown in bold lines. Lighter lines denote county boundaries. Stippling represents urban areas. Triangles denote locations of routine surface meteorological sites used in the development of modeling inputs. Numbers indicate locations of surface monitoring sites used in the Philadelphia Oxidant Study. (Note: sites 6 and CHES; 15 and NEAP; and 3 and BRIS are collocated.)

TABLE 5-1. Routine surface meteorological sites in the vicinity of Philadelphia with data available on 13 July 1977.

Site ID	Site Name	UTM Zone 18 UTMX	UTM Zone 18 UTMY	UAM Modeling Domain x	UAM Modeling Domain y
NEAP	Northeast Philadelphia Airport, PA	499.0	4436.0	22.4	19.2
PIAP	Philadelphia International Airport, PA	478.6	4414.6	18.3	14.9
MCGR	McGuire Air Force Base, NJ	534.1	4431.3	29.4	18.3
WILL	Willow Grove Naval Air Station, NJ	488.7	4449.8	20.3	22.0
LAKH	Lakehurst Naval Air Station, NJ	556.9	4431.5	34.0	18.3
TREN	Trenton Mercer-County Airport, NJ	515.6	4459.0	25.7	23.8
MILL	Millville Airport, NJ	494.3	4357.0	21.5	3.4
WILM	Greater Wilmington Airport, DL	448.6	4390.7	12.3	10.1
CHES	Chester, PA	467.8	4409.3	16.2	13.9
BRIS	Bristol, PA	510.0	4439.5	24.6	19.9
ALGH	Alleghany, PA	499.0	4425.2	22.4	17.0

TABLE 5-2. Routine air quality observation in operation on 13 July 1979 in the vicinity of Philadelphia.

Site ID	Site Number in Figure 5-2	Site Name	Location UTM Zone 18 (km) UTMX	Location UTM Zone 18 (km) UTMY
AMS	1	Air Management Services Laboratory, PA	491.6	4428.5
CAMD	5	Camden, NJ	491.7	4419.0
CHES	6	Chester, PA	469.0	4410.0
CLAY	7	Claymont, DL	461.5	4406.4
FRAN	11	Franklin Institute, PA	485.2	4422.8
SOUT	18	South Broad and Spruce Streets, PA	486.1	4421.6
BRIS	3	Bristol, PA	510.0	4439.0
NEAP	12	Northeast Airport, PA	499.0	4436.0
ANCO	2	Ancora, NJ	511.8	4392.4

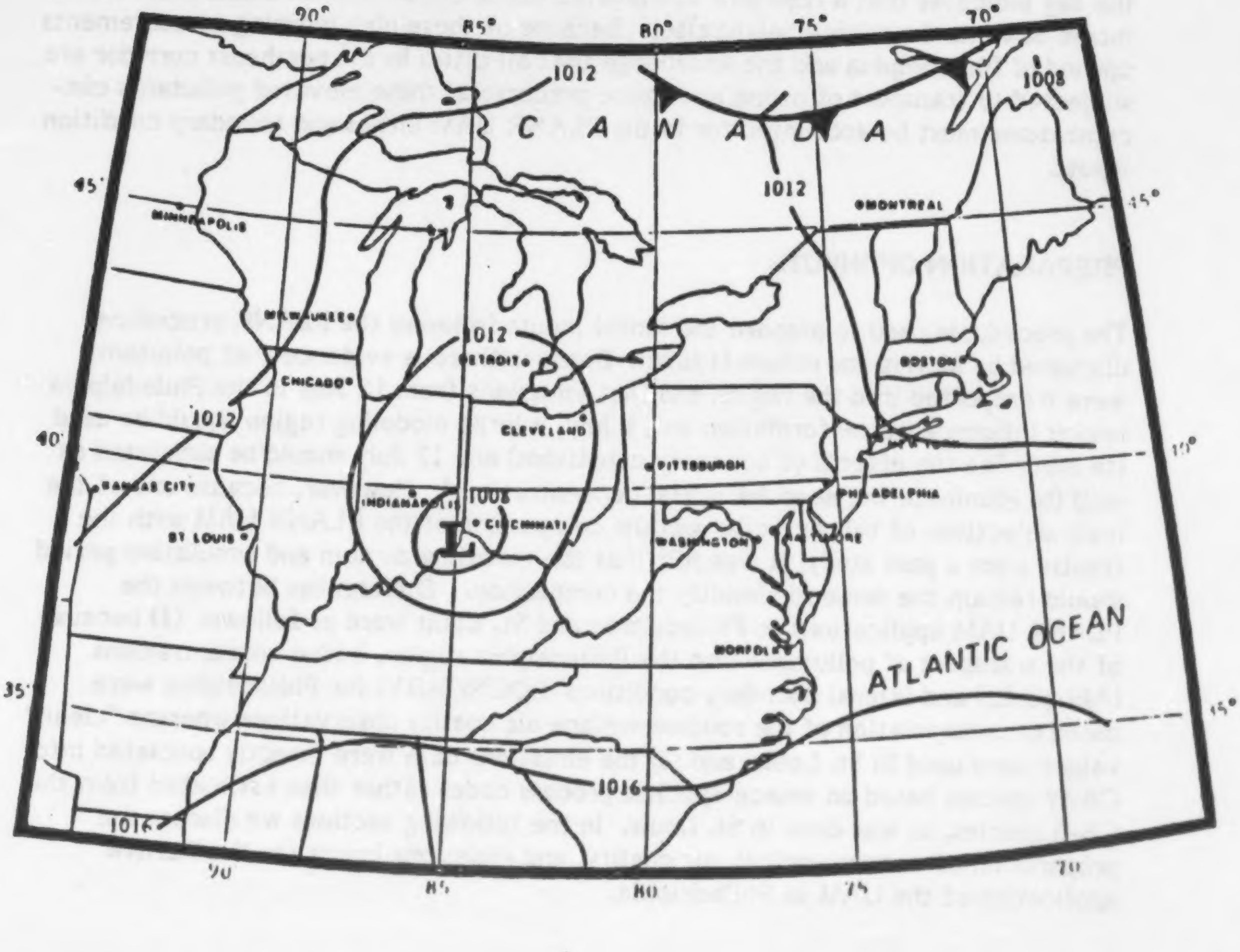
90°
85°
80°
75°
70°
1012
1008
C A N A D A
1012
MONTREAL
45°
45°
MINNEAPOLIS
MILWAUKEE
1012
DETROIT
BOSTON
CHICAGO
1012
CLEVELAND
NEW YORK
40°
40°
KANSAS CITY
PITTSBURGH
PHILADELPHIA
INDIANAPOLIS
1008
CINCINNATI
L
ST LOUIS
WASHINGTON
BALTIMORE
ATLANTIC OCEAN
NORFOLK
35°
35°
1016
1016
90
85
80
75
70

FIGURE 5-3. Synoptic surface weather map at 0700 EST, July 13, 1979.
(Source: Allard et al., 1981)

ozone concentrations at two of the routine sites upwind (north) of the Philadelphia urban core were quite high at 1000 EST on 13 July 1979. Observed ozone concentrations at 1000 EST exceeded 12 pphm at Ancora, New Jersey and exceeded 8 pphm at Bristol, Pennsylvania. The presence of high surface ozone at such an early time of the day indicates that a reservoir of elevated ozone concentration exists aloft and is mixed down as the mixing height rises. Because of these high morning measurements upwind of Philadelphia and the knowledge that all cities in the northeast corridor are subjected to transport of ozone and ozone precursors, these elevated pollutants concentrations must be accounted for in the PLANR UAM initial and boundary condition inputs.

PREPARATION OF INPUTS

The procedures used to prepare the model inputs followed the PLANR procedures discussed by Morris and others (1989c). Because there is evidence that pollutants were transported into the region and that emissions from 12 July in the Philadelphia region influence ozone formation on 13 July, a large modeling region should be used (to minimize the effects of boundary conditions) and 12 July should be simulated as well (to eliminate the need for initial concentrations). However, because one of the main objectives of this exercise was the comparison of the PLANR UAM with the results from a past study, it was felt that the modeling domain and simulation period should remain the same to simplify the comparison. Differences between the PLANR UAM applications to Philadelphia and St. Louis were as follows: (1) because of the transport of pollutants into the Philadelphia region, initial concentrations (AIRQUAL) and lateral boundary conditions (BOUNDARY) for Philadelphia were based on interpolation of the routine surface air quality observations whereas "clean" values were used in St. Louis; and (2) the emissions data were directly speciated into CB-IV species based on source-specific process codes rather than estimated from the CB-II species, as was done in St. Louis. In the following sections we discuss the preparation of meteorological, air quality, and emissions inputs for the PLANR application of the UAM to Philadelphia.

Data Availability

The routine meteorological surface observations sites in operation on 13 July 1979 in the vicinity of Philadelphia are listed in Table 5-1. The locations of these routine sites are shown in Figure 5-2. No routine upper-air observations were available in the immediate vicinity of Philadelphia. Thus we relied on upper-air observations from two sites: (1) Dulles International Airport, approximately 225 km west-southwest of Philadelphia, and (2) John F. Kennedy (JFK) International Airport, approximately 145 km east-northeast of Philadelphia.

Routine surface air quality observation sites consisted of the nine sites within the Philadelphia UAM modeling domain listed in Table 5-2. All nine sites measured hourly average ozone concentrations on 13 July 1979. In addition, three of the sites also measured NO, NO_2, and CO (AMS Laboratory, Camden, and South Broad), and two sites also measured CO (Ancora and Camden).

Although data from only the nine routine air quality monitoring sites were used in the development of the PLANR UAM inputs, 21 air quality observation sites (see Figure 5-2), including 12 from the Philadelphia Oxidant Study (POS) were used in the evaluation of the PLANR UAM.

Model Inputs

DIFFBREAK: Mixing heights in the Philadelphia area were estimated using upper-level temperature soundings at Dulles and JFK airports and hourly surface temperature from the Philadelphia routine surface meteorological monitoring network (Table 5-1) using the method described by Kelley (1981). Calculated maximum mixing heights were 1775 m AGL based on the Dulles Airport soundings and 1881 m AGL based on the JFK Airport soundings. Because JFK Airport is on the coast and Philadelphia and Dulles Airport are further inland, the Dulles mixing height was felt to be more representative of conditions in Philadelphia. The nighttime DIFFBREAK was assumed to be 250 m AGL and the diurnal variation in the mixing height was calculated using the Dulles Airport sounding and the hourly varying surface temperatures. The spatially varying mixing height field was then obtained by using the 1/r interpolation in the UAM preprocessor DFSNBK.

REGIONTOP: The region top for the PLANR application of the UAM to Philadelphia was defined as 1850 m AGL. This value is 75 m above the maximum mixing height; thus all five vertical layers are assumed to lie within the mixing layer during the period of the maximum mixing height.

WIND: The Diagnostic Wind Model (DWM) was configured for 14 layers. Surface wind data were taken from the 11 routine sites and upper-air wind soundings from Dulles and JFK airports. Because Philadelphia was approximately between the two upper-air sites, the hourly domain-mean vertical wind sounding needed as input to the DWM was calculated by averaging the soundings from Dulles and JFK and using linear interpolation between the average morning and evening soundings to the hour of interest.

Two wind fields were prepared for the Philadelphia region, one each for diagnostic runs 1 and 2. In diagnostic run 1 the wind observations were used without adjustments. For diagnostic run 2 the surface wind speeds at the instantaneous FAA/NWS sites (all six surface sites) were used but reduced by 50 percent. The two wind fields generated for the diagnostic runs are shown in Appendixes B and E, respectively.

METSCALERS: The NO_2 photolysis rates (RADFACTOR) were calculated from the solar zenith angle and assuming clear skies; the procedures described by Schere and Demerjian (1977) and actinic flux data collected by Bass and co-workers (1980) were used. Exposure class was also estimated from the amount of solar radiation, assuming clear skies. Water vapor concenrations were calculated from the hourly dew point measurements recorded at Philadelphia International Airport. Water vapor concentrations were approximately 17,000 ppm in the morning of 13 July 1979. At around 0600 EST water vapor concentrations started rising and peaked at approximately 27,000 ppm at 1300 EST. By 2000 EST the concentration of water vapor was about 20,000 ppm.

The values for temperature gradients below the diffusion break (TGRADBELOW) and above (TGRADABOVE) were estimated from the JFK Airport temperature soundings (see Figure 5-4) and the calculated mixing heights. The values used for metscalers are given in Table 5-3.

AIRQUALITY: The initial conditions at 0000 on 13 July 1979 for the first two layers of the UAM, which lie below the diffusion break, were estimated by using 1/r interpolation of the measurements (i.e., O_3, NO, NO_2, and CO) from the nine routine air quality sites and four hypothetical stations located at the four corners of the modeling domain with assumed "clean" values. Since no measurements of VOC were available, the initial concentration of VOC was assumed to be "clean" (0.025 ppmC) for the two layers below the diffusion break (250 m AGL). Other species concentrations in the CB-IV mechanism were set to their minimum value, either 0.000001 or 0.0000000001 ppm. Initial concentration in the three layers above the diffusion break were assumed to be "clean" as defined in Section 3.

BOUNDARY: Because of the stagnant recirculation conditions of 13 July 1979 and the short simulation period (0000 to 2000), boundary concentrations do not greatly influence calculated ozone formation on 13 July 1989. Accordingly, the boundary conditions used in a previous UAM application to Philadelphia (Haney and Braverman, 1985) were also used here to simplify the comparison with that study (see Chapter 6).

TOPCONC: Because no routine air quality data were measured aloft in the Philadelphia region on 13 July 1979, boundary concentrations above the region top were assumed to be the same "clean" values used for St. Louis (Section 3).

TEMPERATUR: The gridded field of hourly varying surface temperatures was obtained by using 1/r interpolation from the surface measurements from the routine network (Table 5-1).

EMISSIONS and PTSOURC: The original emission inventory developed for the EPA by Engineering-Science (EPA, 1982) was obtained on magnetic tape in the form of disaggregated raw data files containing information for major point, minor point, mobile, and area source emissions. These files were then processed with the emission preprocessor CENTEMS (see SAI, 1989) to obtain a gridded low-level emission

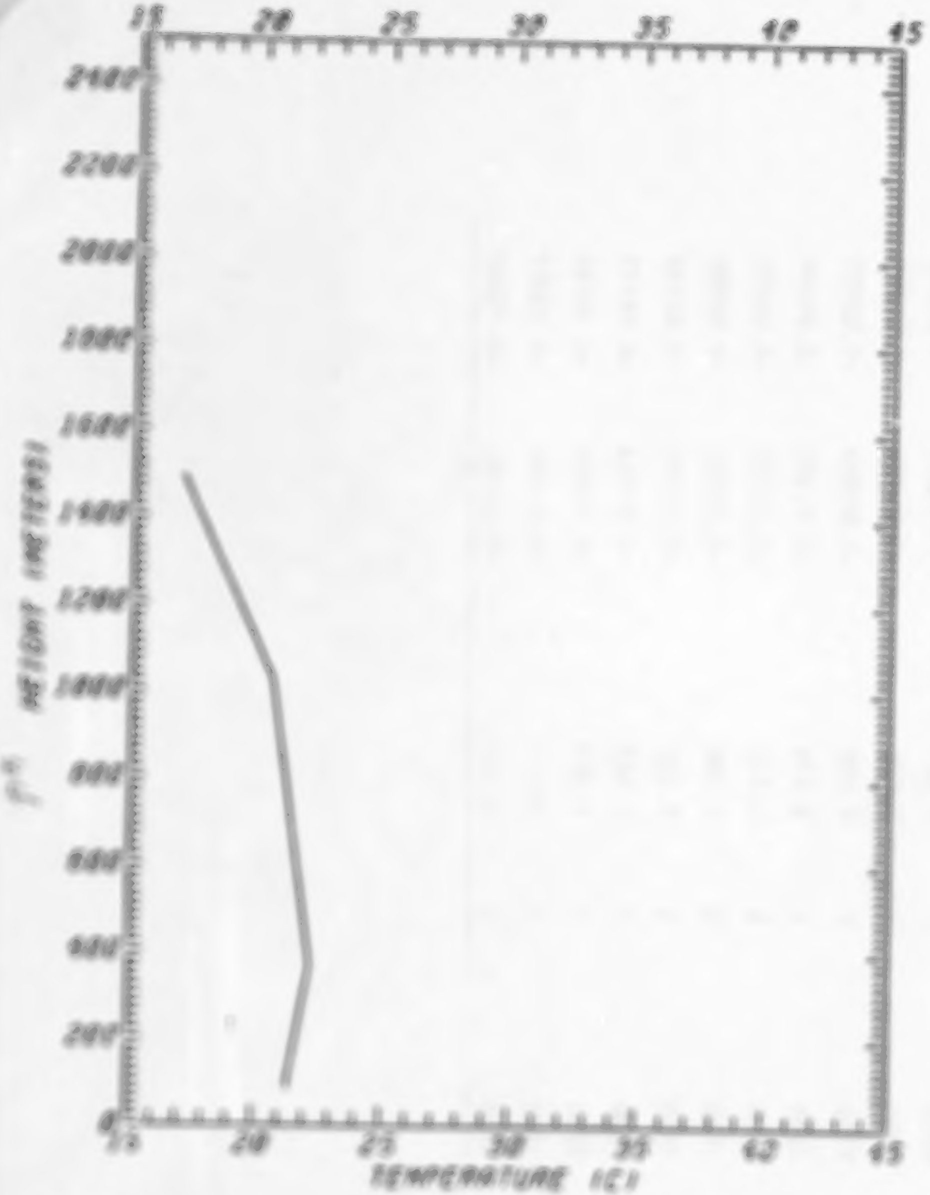

FIGURE 5-4a. Temperature sounding for Dulles airport on 13 July 1978—0700 EDT. (Source: Haney and Braverman, 1985)

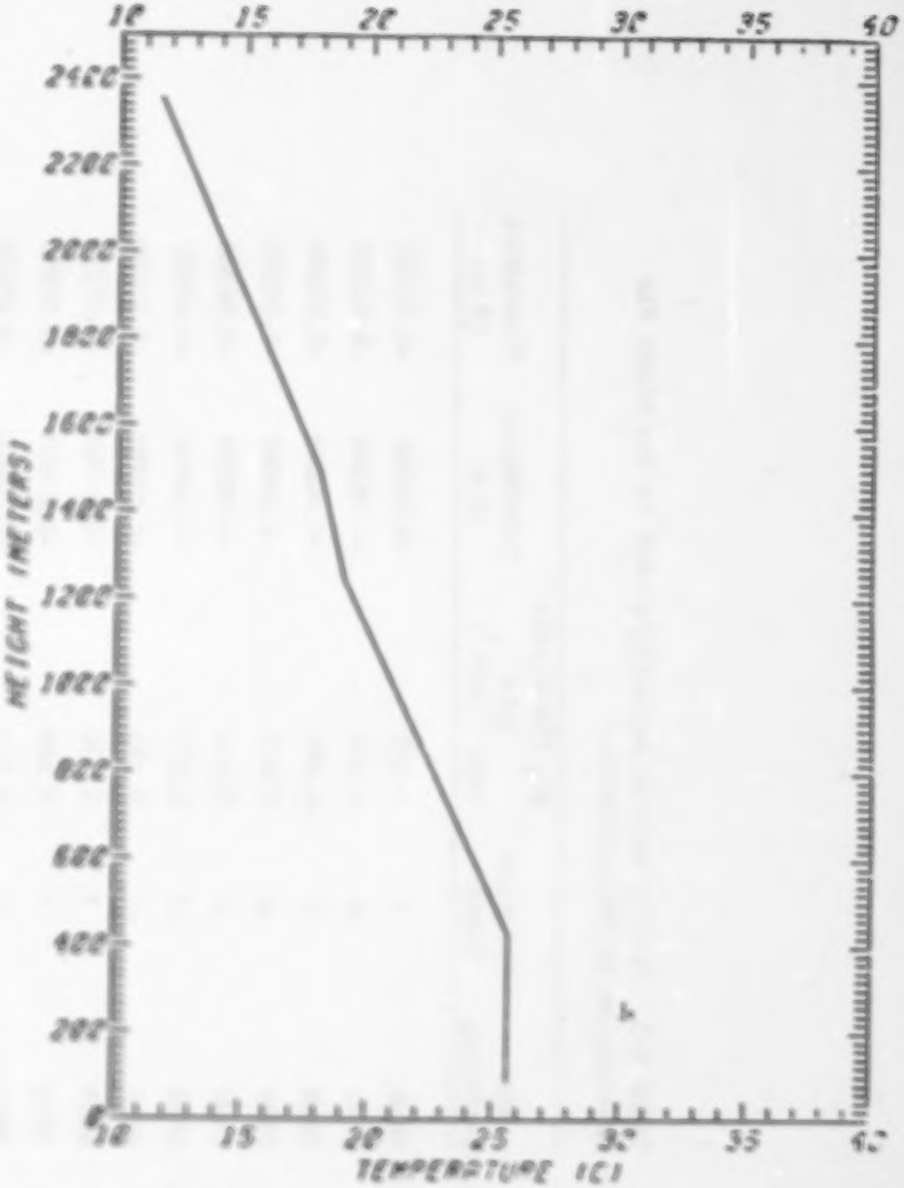

FIGURE 5-4b. 1900 EDT.

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TABLE 5-3. Hourly varying metscalars used in the PLANR UAM application to Philadelphia.

Hour Beginning	Exposure Class	NO_2 Photolysis Rate (ppm^{-1} min^{-1})	TGRADBELOW (K/m)	TGRADABOVE (K/m)
0000	-2	0.000	-0.00040	-0.00380
0100	-2	0.000	-0.00040	-0.00380
0200	-2	0.000	-0.00040	-0.00380
0300	-2	0.000	-0.00040	-0.00380
0400	-2	0.000	-0.00040	-0.00380
0500	-2	0.018	-0.00040	-0.00380
0600	-2	0.160	-0.00750	-0.00380
0700	1	0.230	-0.01000	-0.00218
0800	1	0.444	-0.01000	-0.00256
0900	2	0.523	-0.01050	-0.00286
1000	2	0.576	-0.01050	-0.00240
1100	2	0.608	-0.01050	-0.00127
1200	3	0.619	-0.01050	-0.00040
1300	3	0.612	-0.01050	-0.02950
1400	3	0.586	-0.01050	-0.02950
1500	3	0.530	-0.01050	-0.02950
1600	2	0.457	-0.01050	-0.05117
1700	2	0.363	-0.01050	-0.10000
1800	1	0.211	-0.01000	-0.12667
1900	1	0.059	-0.01000	-0.12667

file (EMISSIONS) and elevated emission file for a typical summer weekday with speciation of hydrocarbons appropriate to CB-IV. No adjustment (e.g., temperature effects) to the emissions on 13 July 1979 was made. The elevated emission file contains emissions rates and stack parameters for major point sources; this file is used as input, along with the UAM meteorological inputs, in the point source preprocessor to obtain the UAM elevated emissions file PTSOURC.

The spatial distributions of the low-level NO_x and VOC emissions are shown in Figures 3-5 and 3-6. Table 3-6 lists the emission totals for NO_x and VOC for both the low-level emissions (EMISSIONS) and elevated emissions (PTSOURC) input files. Also shown in Table 3-6 are the emission totals used in the earlier UAM/CB-II modeling study for Philadelphia (Haney and Braverman, 1985). The emission totals for the two studies differ because the source-specific or process-specific VOC and NO_x factors used to split the VOC and NO_x species are different in the two versions of the chemical kinetics mechanism (CB-IV or CB-II) and because new updated speciation splits were used in this study. In addition, we used a different definition of when a point source is treated as a low-level source.

DIAGNOSTIC SIMULATIONS TO ARRIVE AT A BASE CASE

We performed two diagnostic simulations for the PLANR application of the UAM to Philadelphia. These diagnostic simulations differed in the observed surface wind speeds used in the UAM wind preprocessor (the DWM). Because of the large amount of ozone and ozone precursors transported into cities in the northeastern U.S. like Philadelphia, and the fairly complex meteorological conditions in Philadelphia on 13 July 1979 (a large amount of wind shear was evident), Philadelphia may not be amenable to the PLANR use of the UAM. More comprehensive measurement studies or modeling, such as the Regional Oxidant Modeling for Northeast Transport (ROMNET) program, are needed to characterize transport in northeastern cities. Thus it was not surprising that the model performance goal—the predicted region-wide maximum ozone should be within 20 percent and in the general vicinity of the observed peak, and the predicted peak ozone at the location of the observed peak should be within 20 percent—could not be met in Philadelphia in only two diagnostic simulations.

Diagnostic Run 1

In the first diagnostic run for Philadelphia the routine meteorological and air quality observations were used in the UAM preprocessors with no adjustments and the model was exercised from 0500 to 1900 on 13 July 1979. The layer 1 wind fields for diagnostic run 1 are shown in Appendix B. Isopleths of predicted hourly ozone concentrations for diagnostic run 1 are shown in Appendix C. Time series of predicted and observed hourly ozone concentrations are in Figure 3-7 and isopleths of predicted daily maximum ozone concentrations are shown in Figure 3-8.

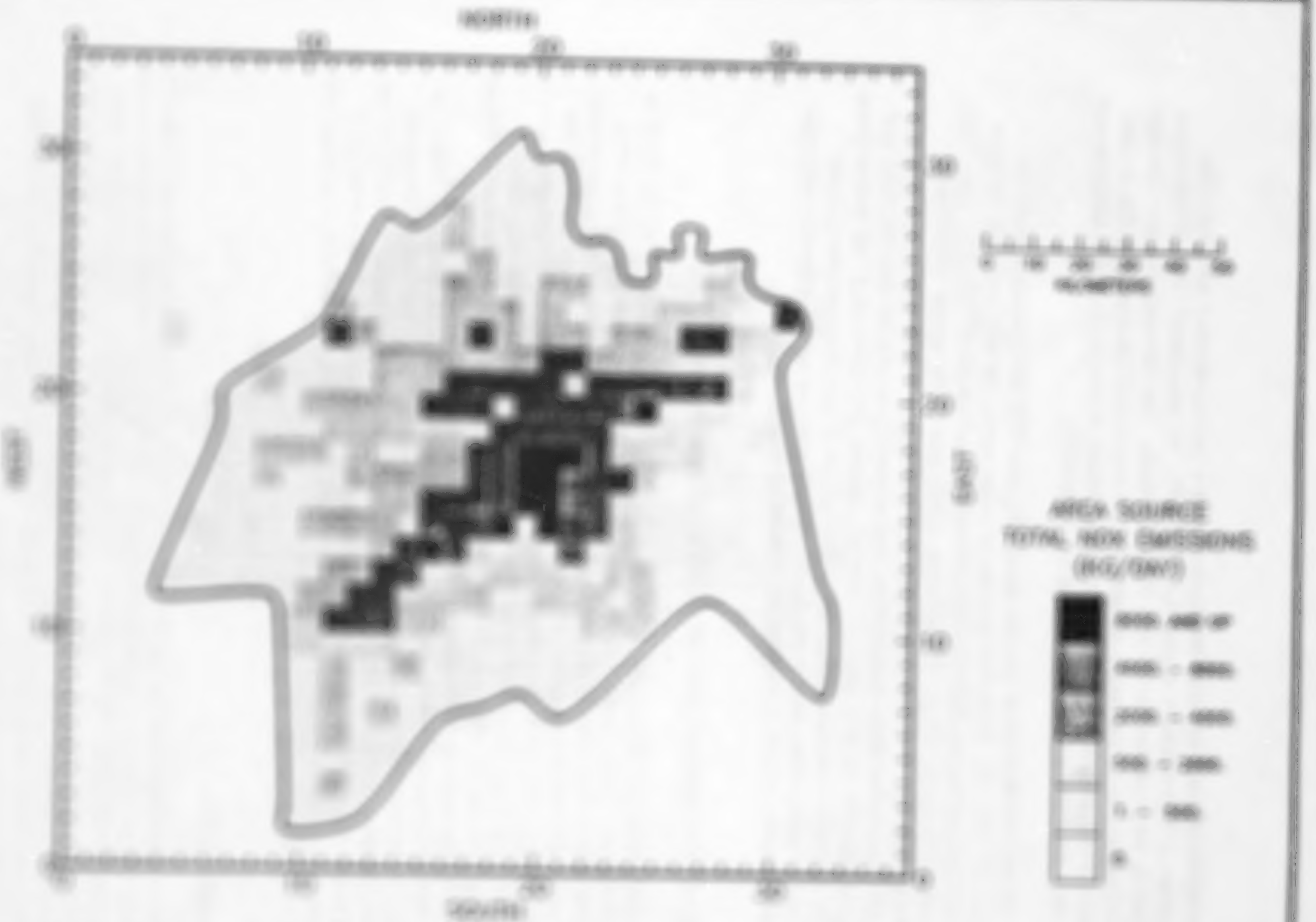
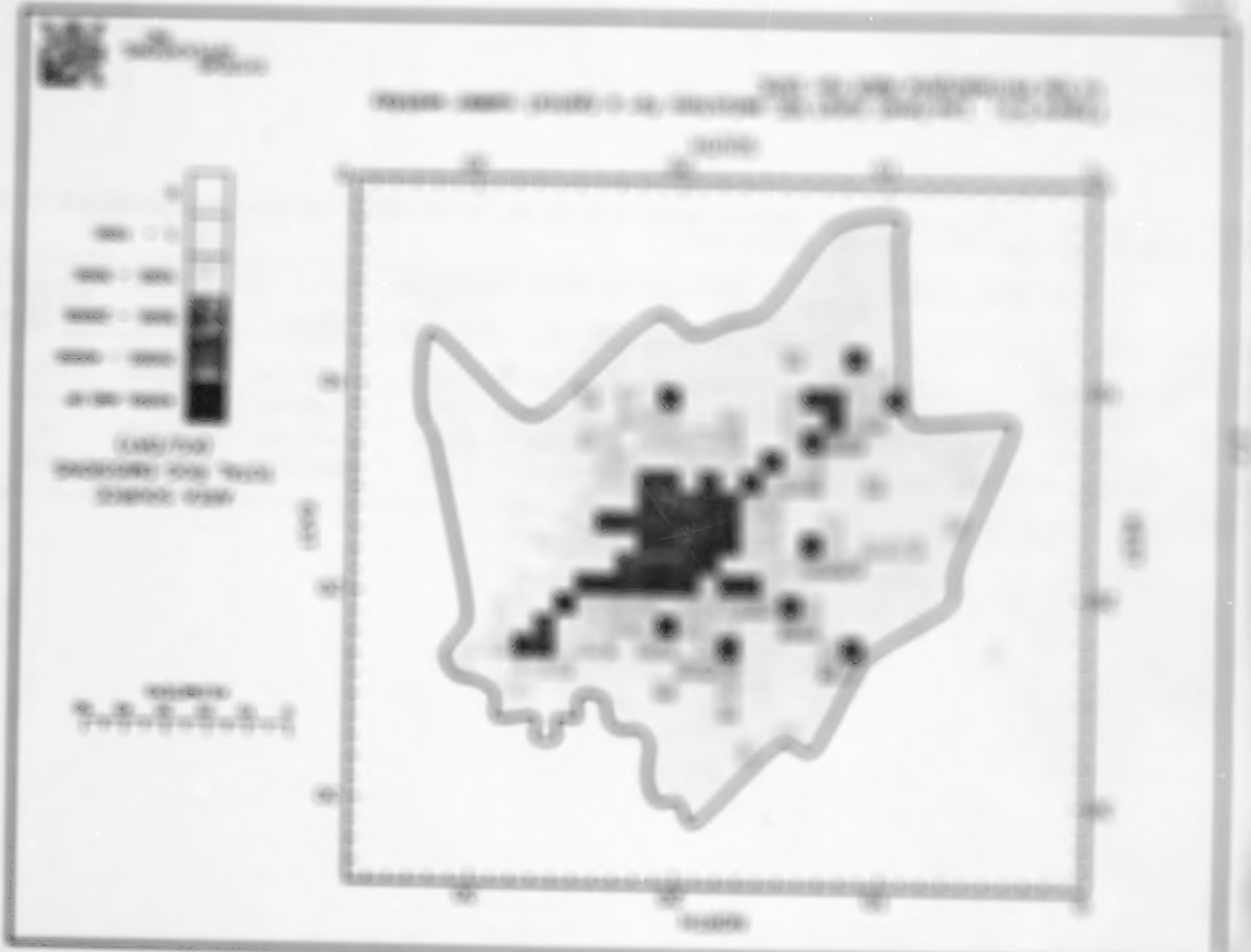

NORTH
SOUTH
WEST
EAST
KILOMETERS
0 10 20 30 40 50
AREA SOURCE
TOTAL NOX EMISSIONS
(KG/DAY)
6000 AND UP
4000 – 6000
2000 – 4000
500 – 2000
0 – 500
0

Figure [illegible]. Low-level NO_x emissions for a typical summer weekday in the [illegible]



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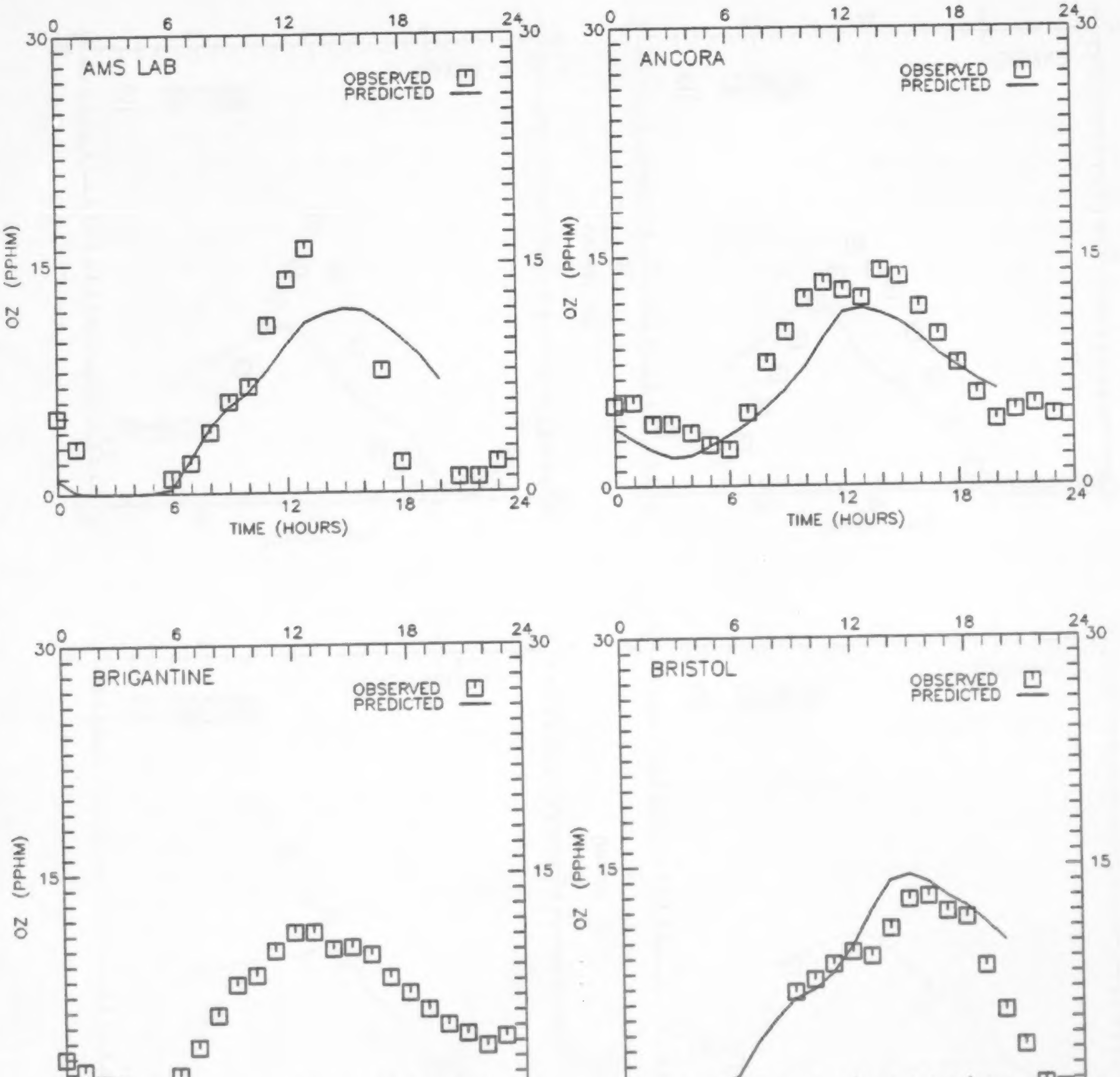


FIGURE 5-7. Time series of predicted and observed hourly ozone concentrations (pphm) in Philadelphia for diagnostic run 1.

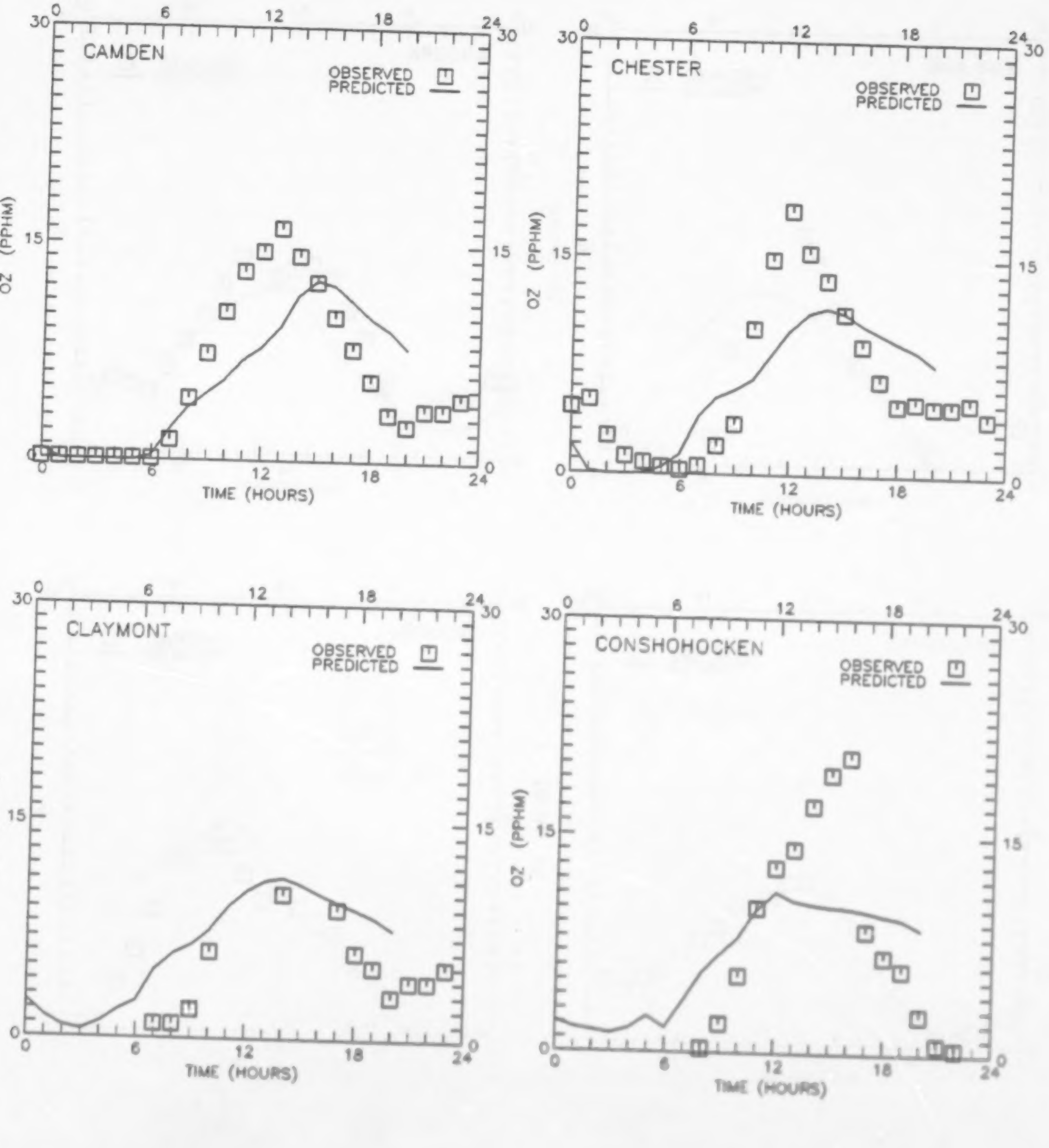


FIGURE 5-7. Continued.

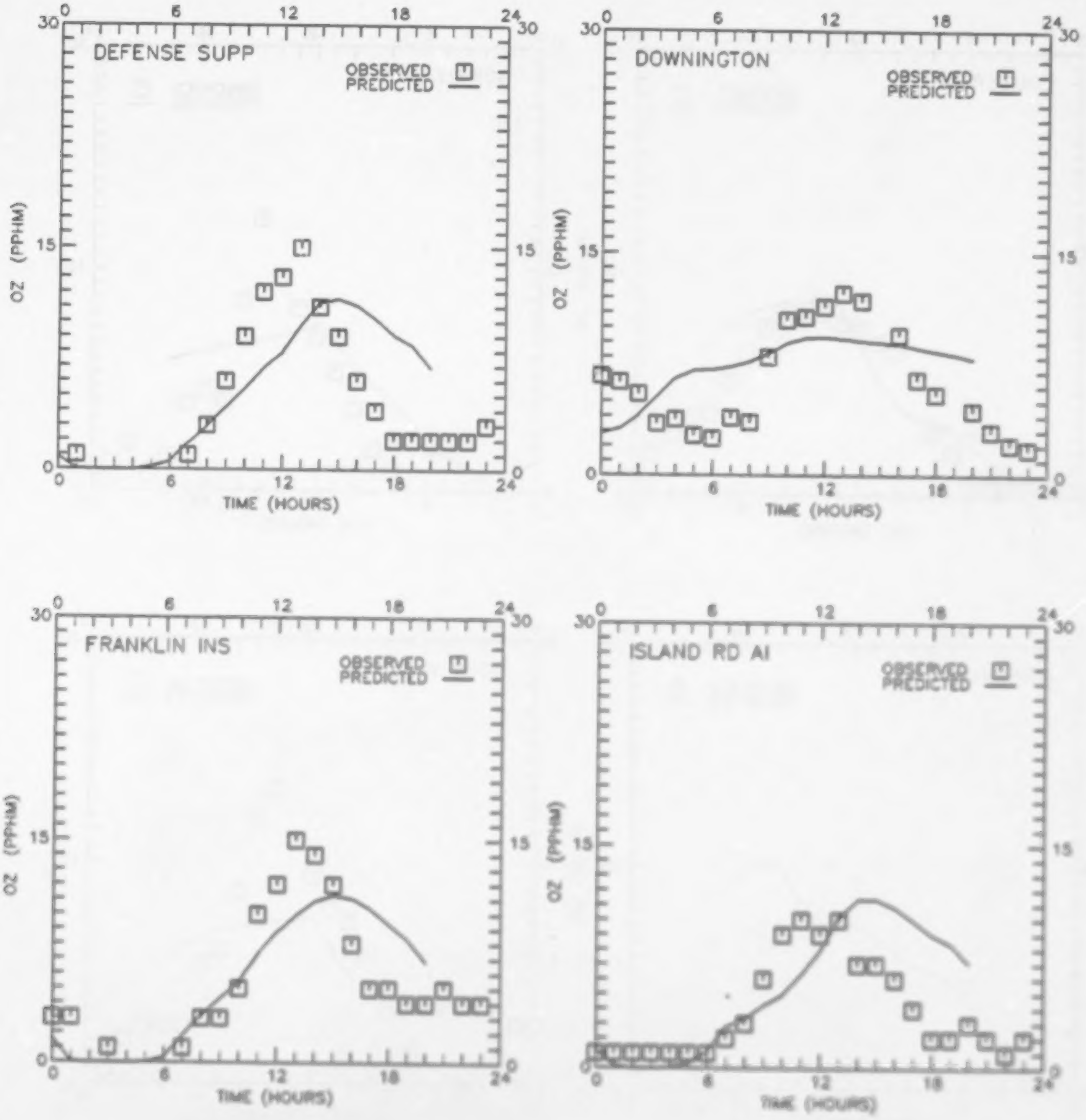


FIGURE 5-7. Continued.

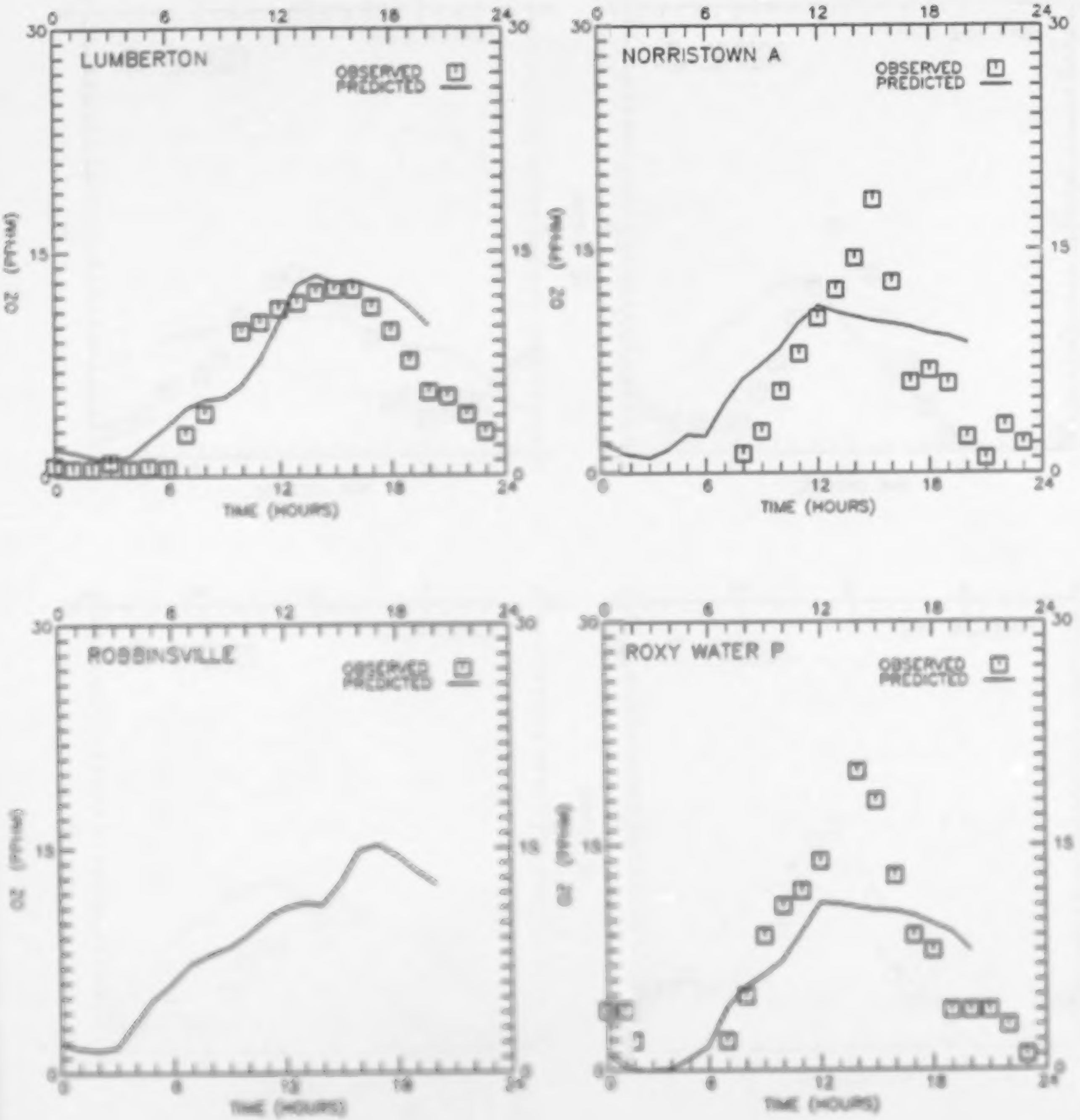


FIGURE 5-7. Continued.

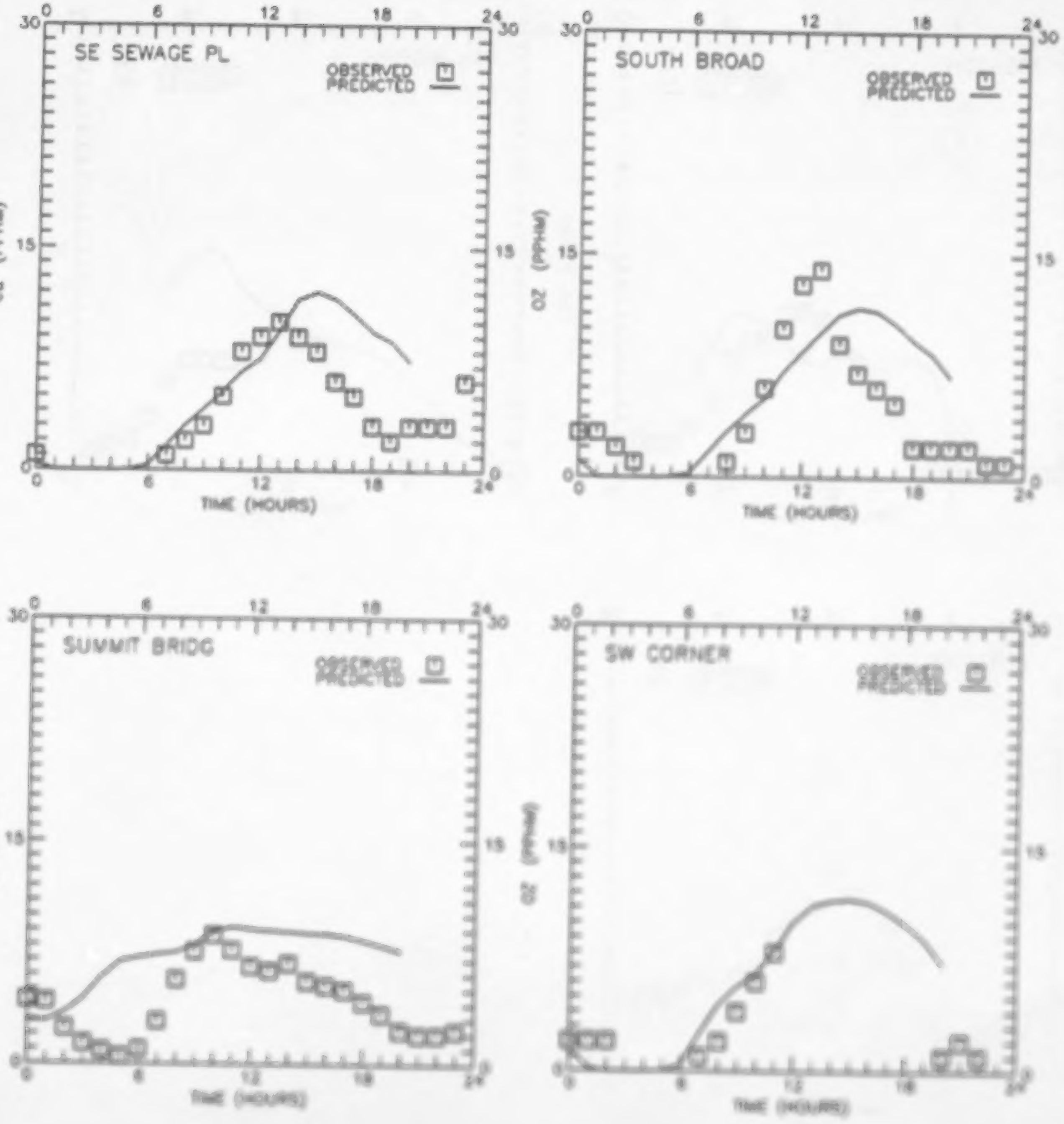


FIGURE 5-7. Continued.

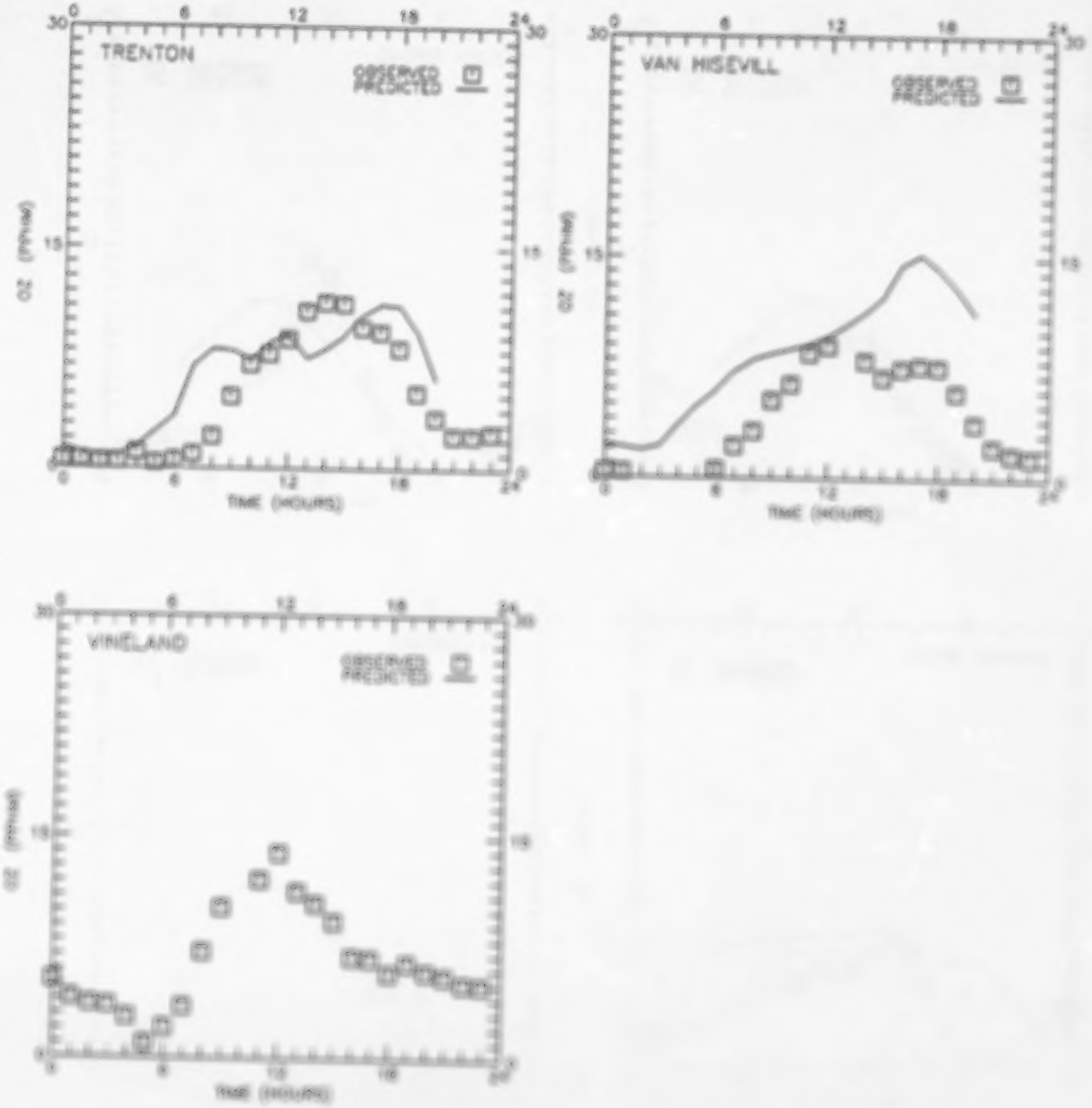


FIGURE 5-7. Concluded.

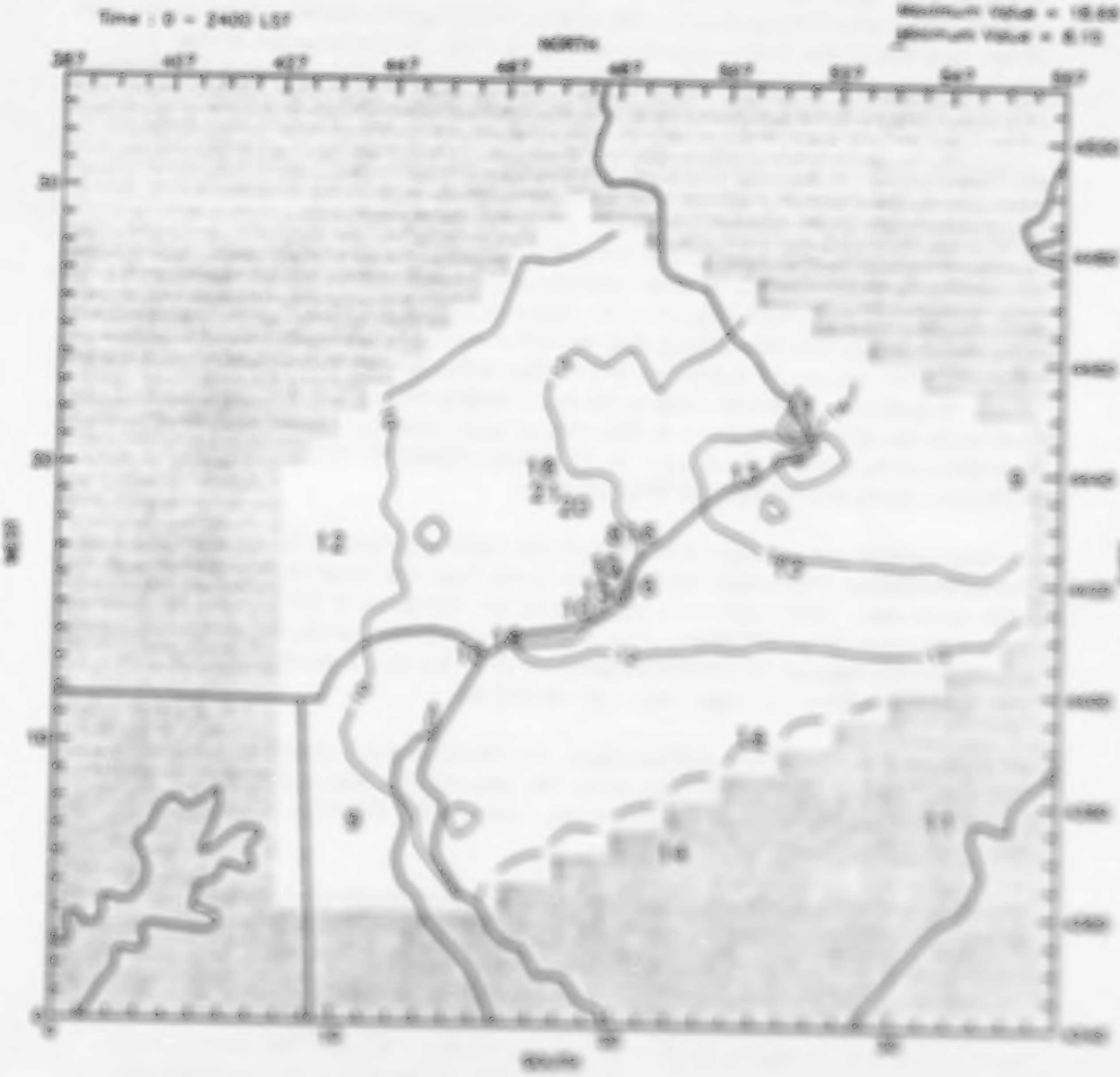

Time : 0 = 2400 LST
Maximum Value = 19.00
Minimum Value = 8.10
NORTH
SOUTH
WEST
EAST
12
9
18
21
20
11
14
16

FIGURE 5.6. Isopleths of predicted daily maximum ozone concentrations (pphm) from Diagnostic Run 1 with superimposed observations.

The predicted region-wide maximum ozone concentration (18.7 pphm) is within 9 percent of the observed peak (20.5 pphm) and occurs approximately 43 km to the east of the location of the observed peak (see Figure 3-8). At the location of the observed peak ozone (Conshohocken) the predicted maximum daily ozone concentration (11.1 pphm) is only within 46 percent of the observed peak.

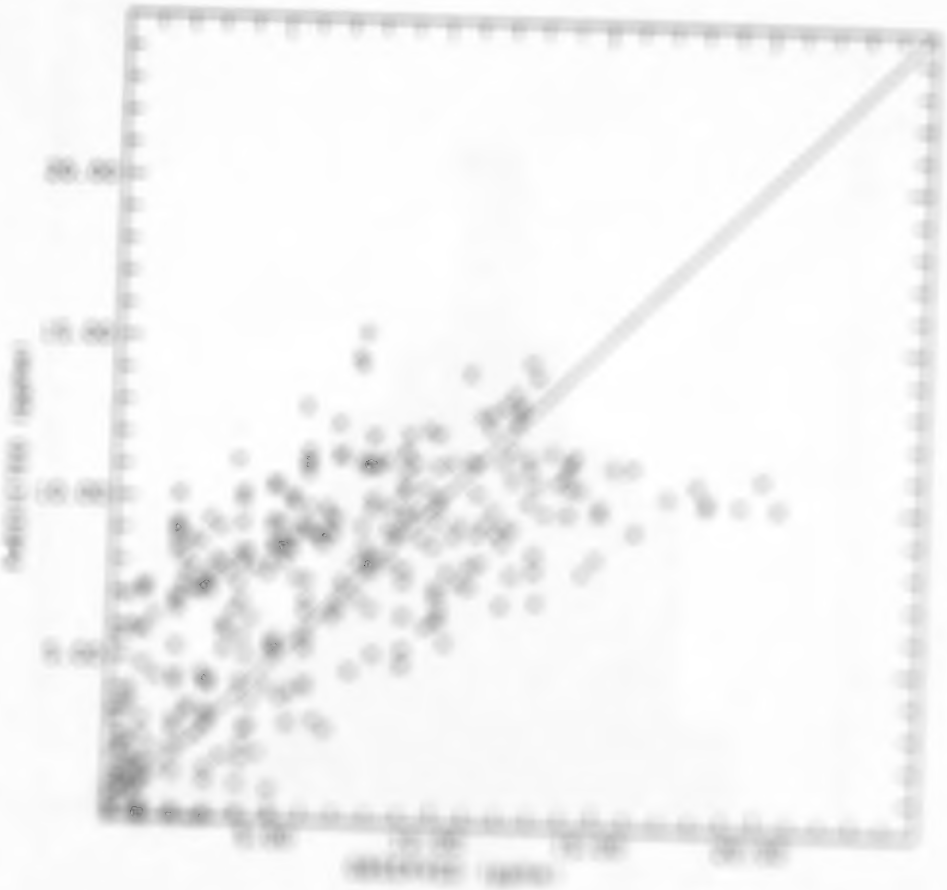
As seen in the time series plots of predicted and observed hourly ozone concentrations for diagnostic run 1 (Figure 3-7), the model does a good job in replicating the observed hourly ozone concentrations in areas far southeast of downtown (Ancora), to the southwest of downtown (Claymont and Summit Bridge), far east of downtown (Lumberton), and northeast of downtown (Bristol and Trenton). At the downtown sites in Philadelphia (AMS Lab, Camden, Defense Support, Franklin Institute, Island Rd., South Broad, and SW Corner) diagnostic run 1 usually underpredicts the peak observed daily maximum ozone concentrations, although this underprediction is well within 30 percent. However, diagnostic run 1 underpredicts the observed daily maximum ozone concentrations at the area of peak observed ozone concentrations (the three sites north of downtown) by 43 percent (Roxy Water), 46 percent (Conshohocken), and 40 percent (Norristown).

At most sites in the vicinity of downtown the model predictions do not rise as fast as the observations; thus predicted peaks are lower than the observations and occur later in the day. There are many possibilities for the delay in the rise of the predictions including: (1) insufficient ozone and ozone precursors aloft are entrained as the mixing height rises or (2) photochemistry early in the day is insufficient because VOC concentrations are lower than they should be.

At sites northeast of Philadelphia, where the highest ozone concentrations were observed, the same problems exist as for the downtown sites, except that around 1200 the wind fields used in diagnostic run 1 advect the elevated ozone cloud eastward away from the observation sites.

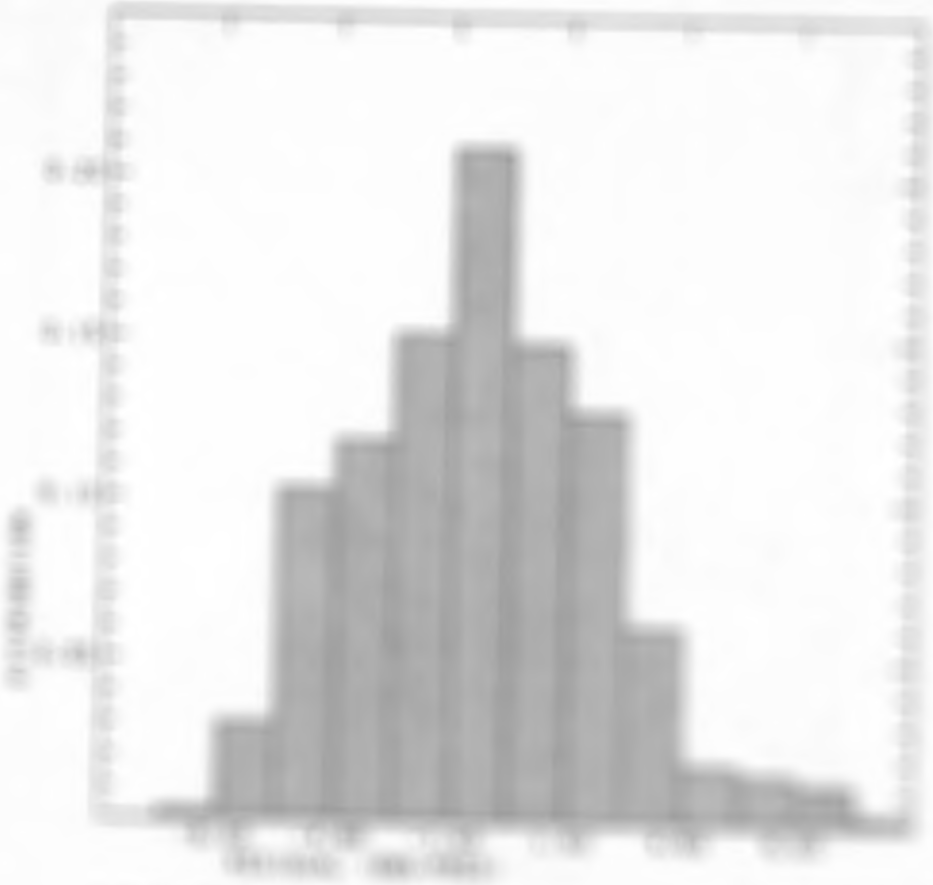
A scatterplot of predicted and observed hourly ozone concentrations and model performance statistics for diagnostic run 1 are given in Figure 3-9. When all hours are considered, the underprediction in the peak observations is compensated for by the overprediction of the low nighttime observations, resulting in an overprediction bias of 13 percent (0.8 pphm). The average absolute (gross) error is about 33 percent (3.0 pphm). The model replicates some of the diurnal variability of the hourly ozone observations, with a correlation coefficient of 0.69; however, the predicted daily maximum ozone concentrations occur later in the day than the observed ozone peaks (Figure 3-7).

Time series of predicted and observed hourly NO, NO$_x$, and CO concentrations for diagnostic run 1 are shown in Appendix B. The model usually follows the trends of the observed NO and NO$_2$ concentrations but has a tendency to underpredict. CO


20.000
15.000
10.000
5.000
5.00
10.00
15.00
20.00

[illegible]

[illegible]



[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

[illegible]

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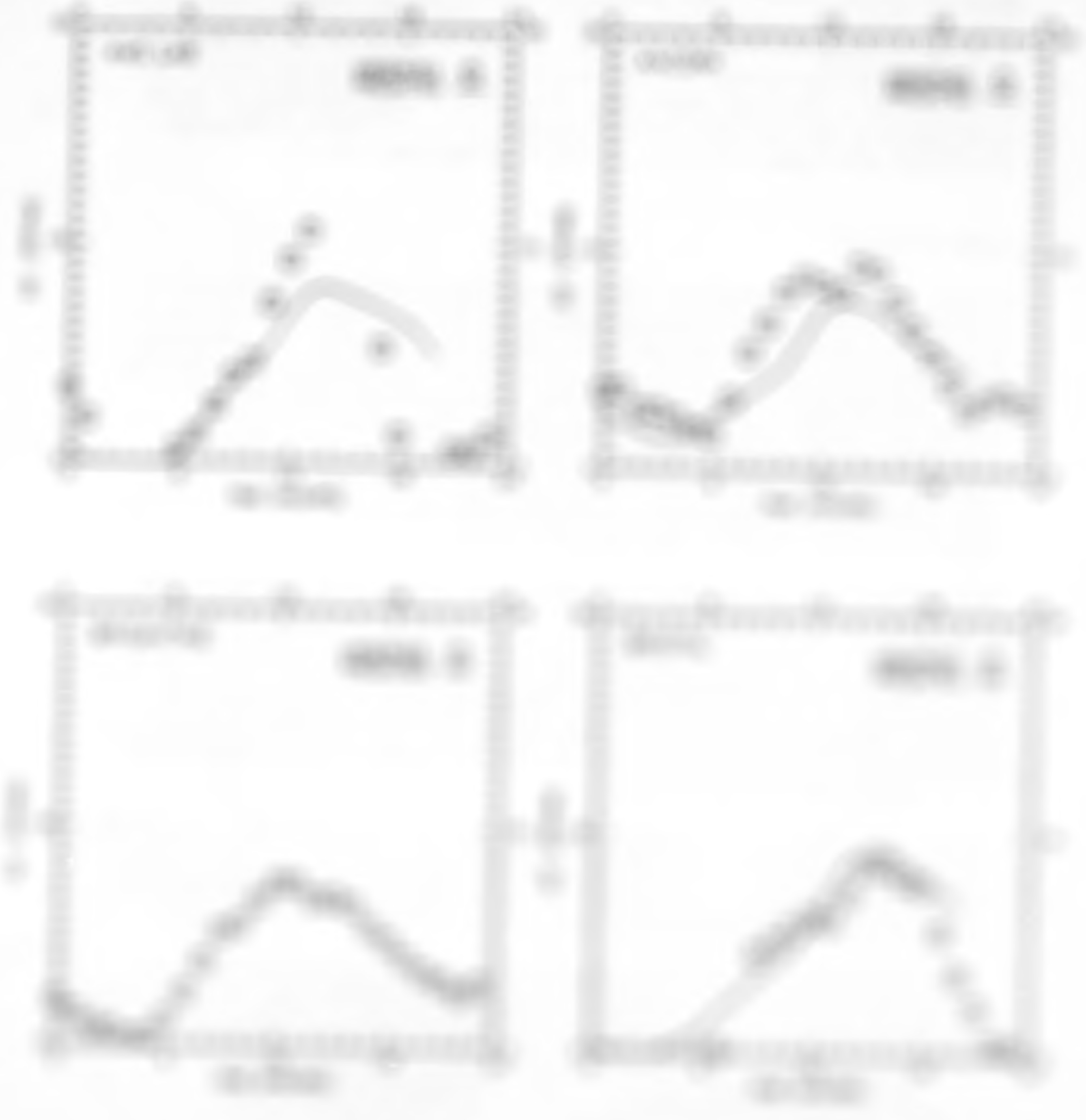
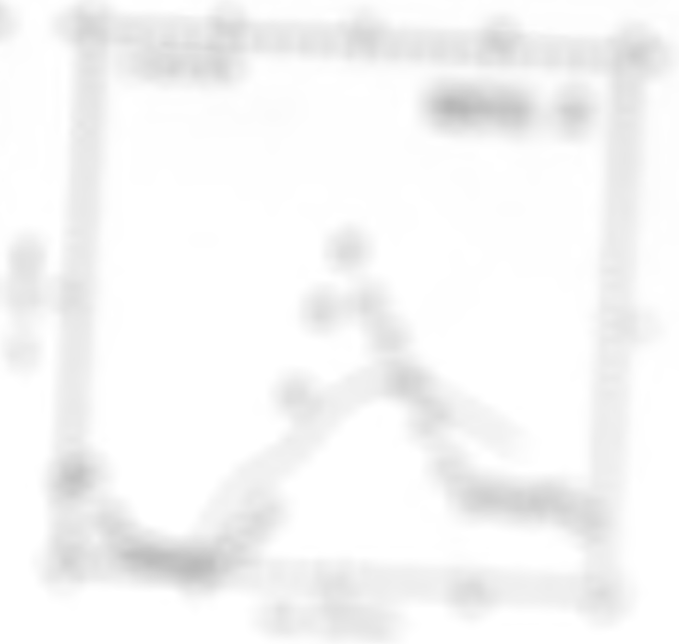
[illegible]

[illegible]

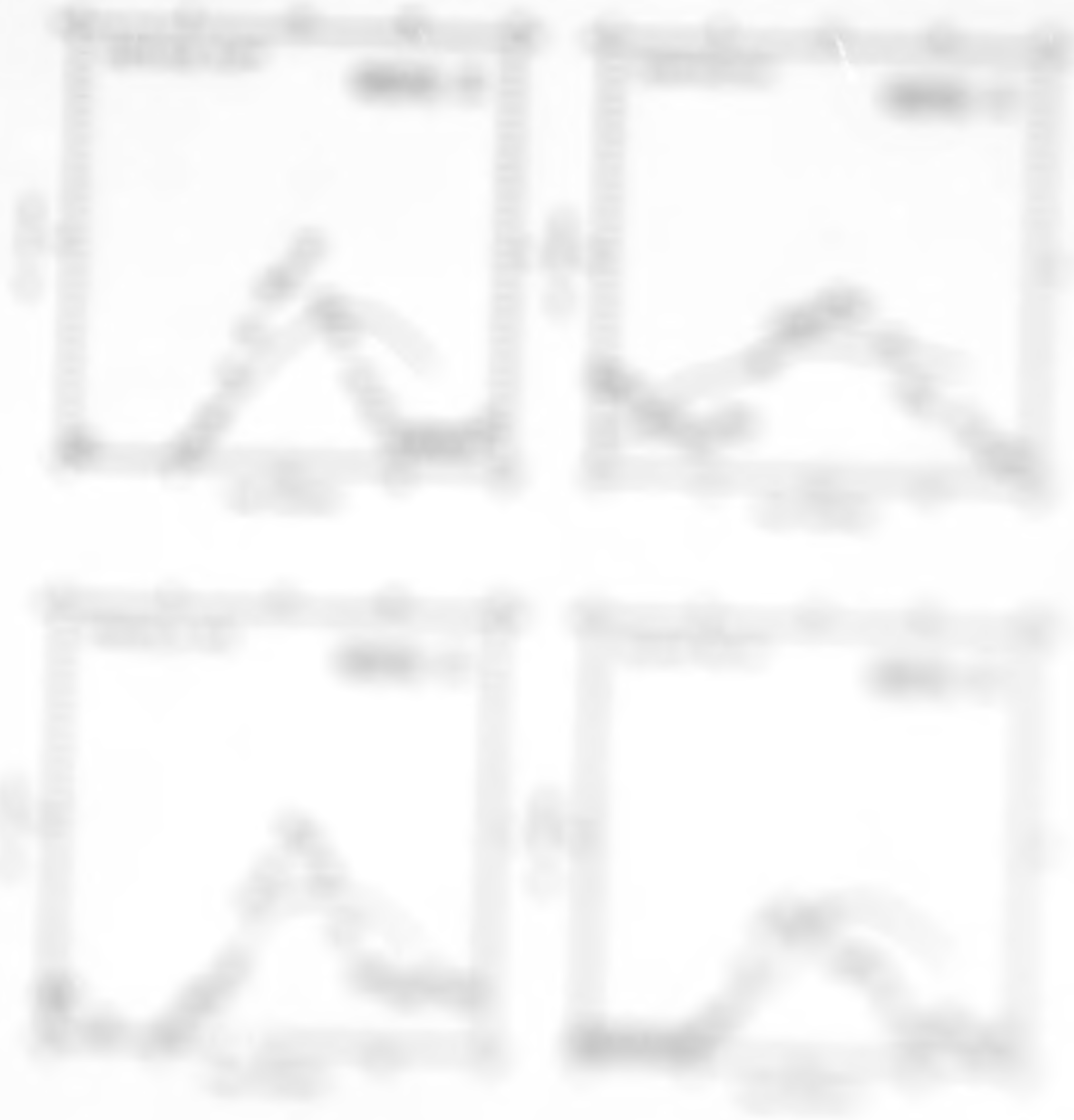
[illegible]



[illegible]



[illegible]



[illegible]

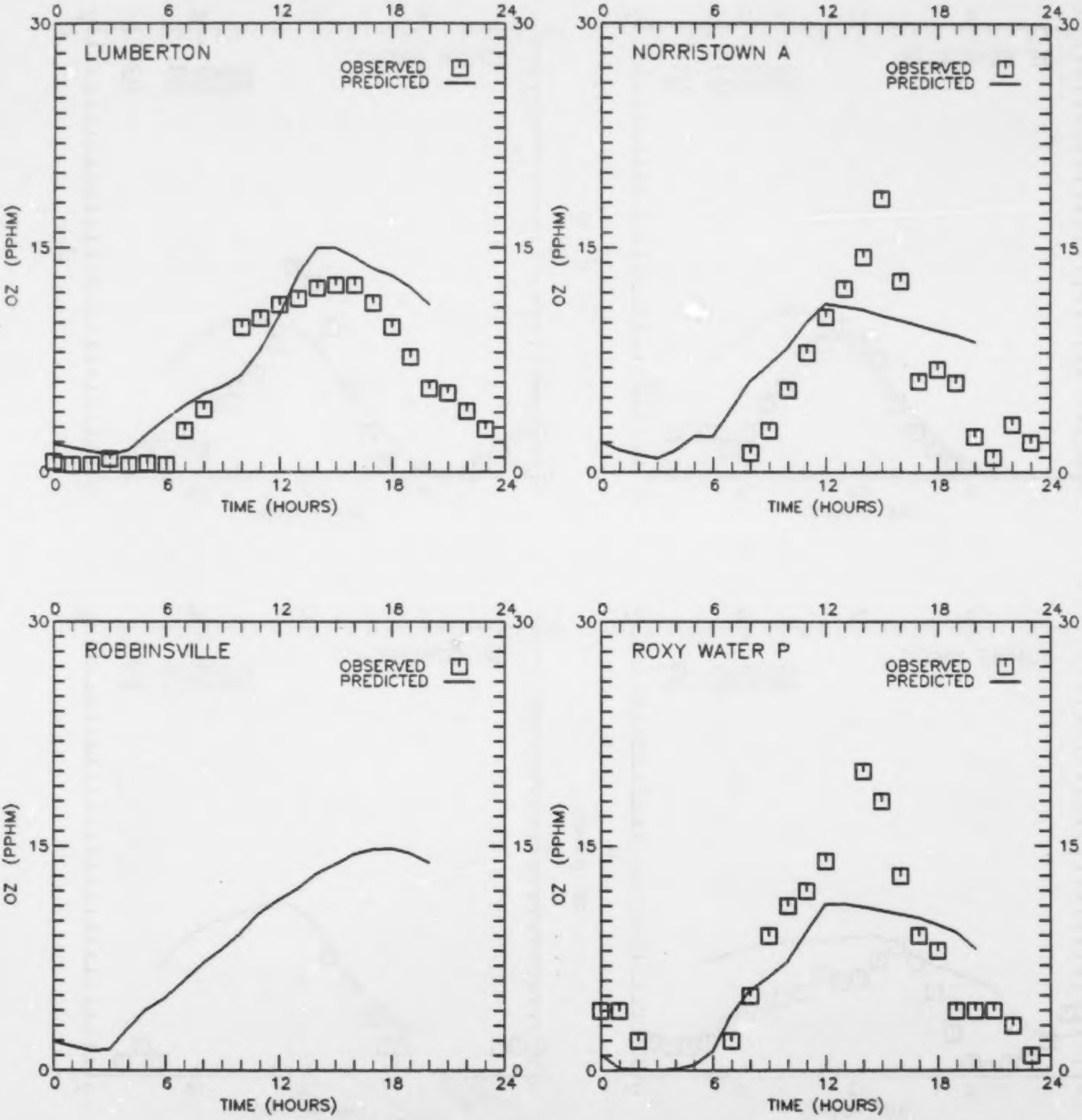


FIGURE 5-10. Continued.

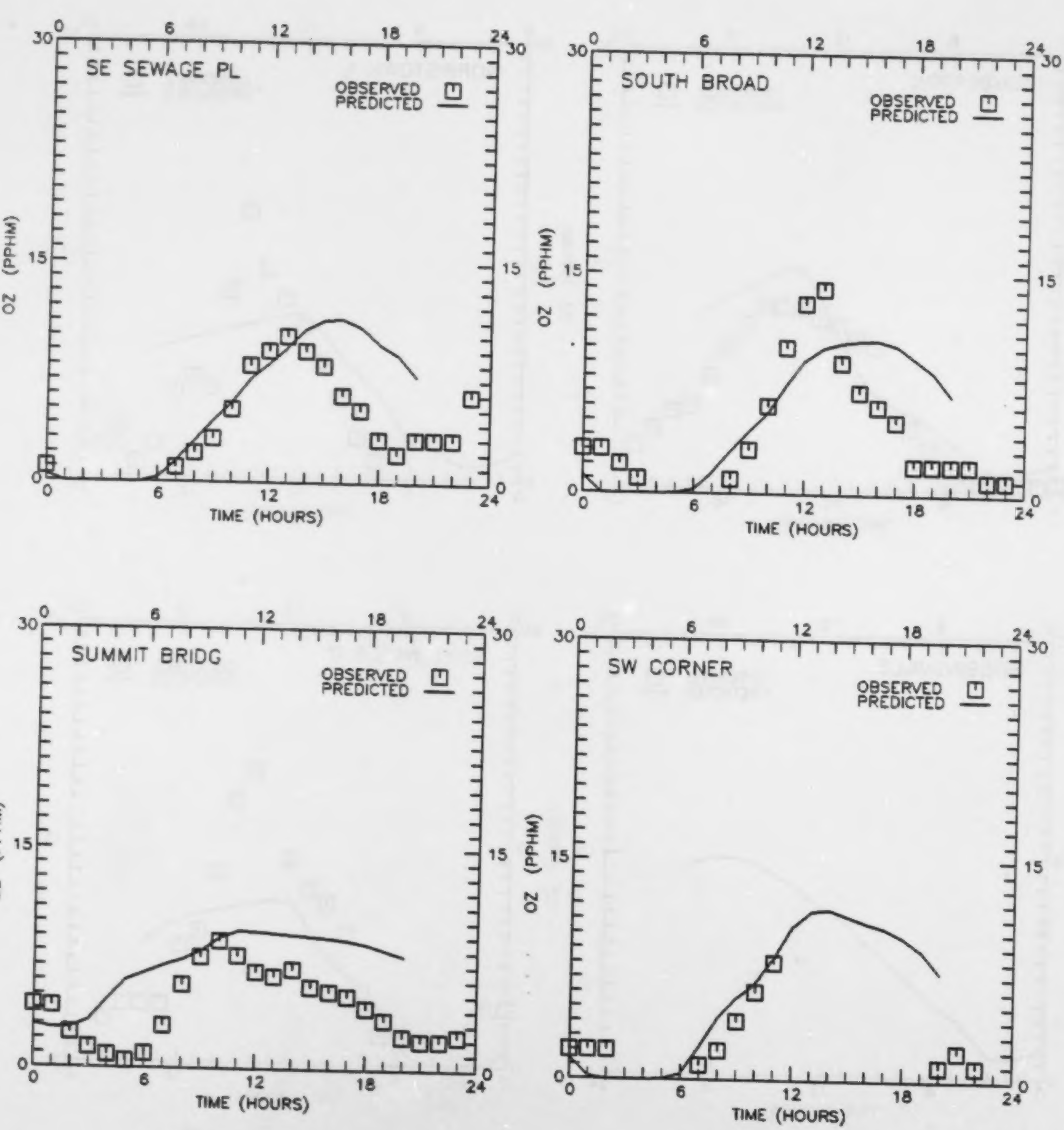


FIGURE 5-10. Continued.

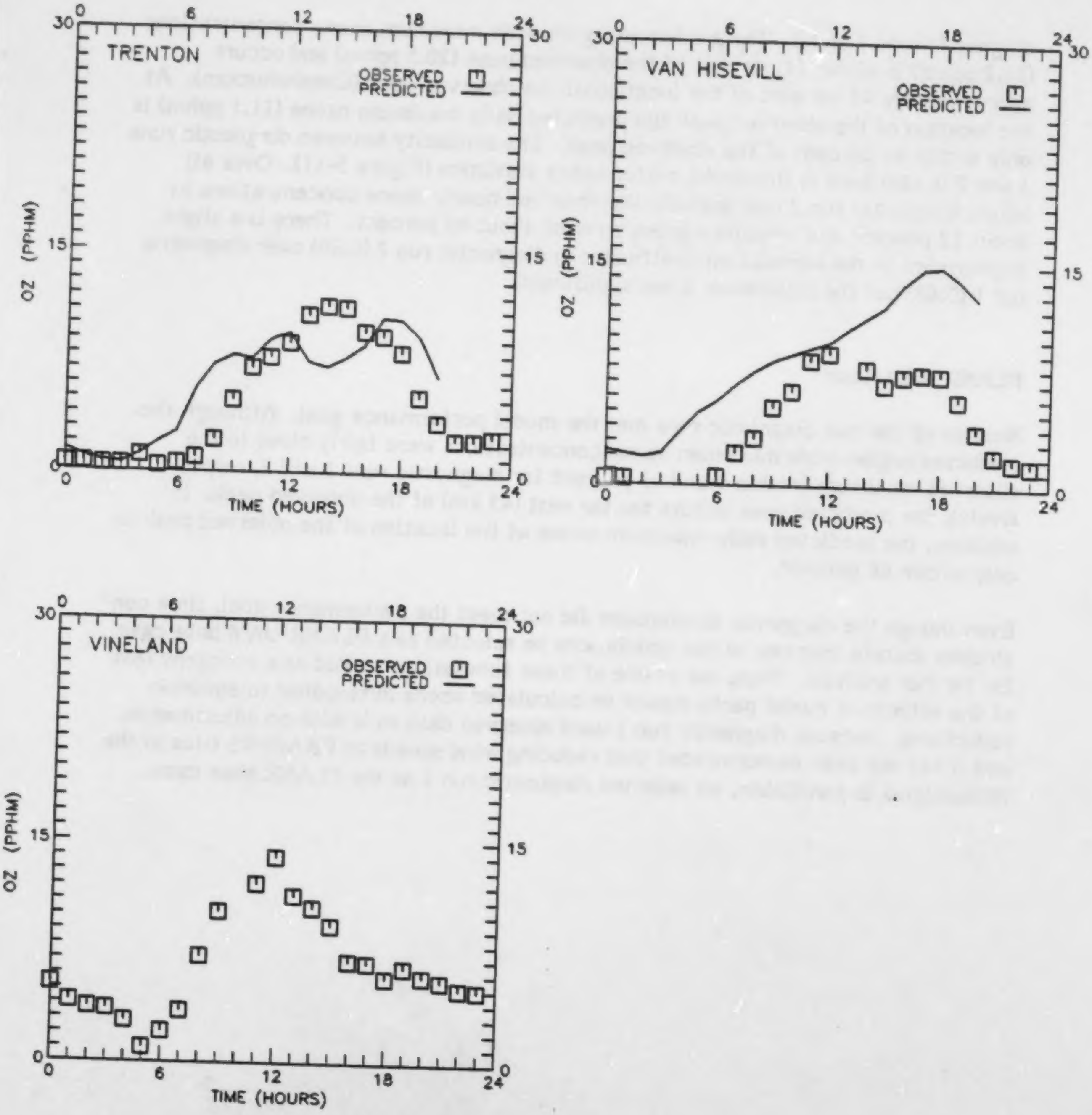


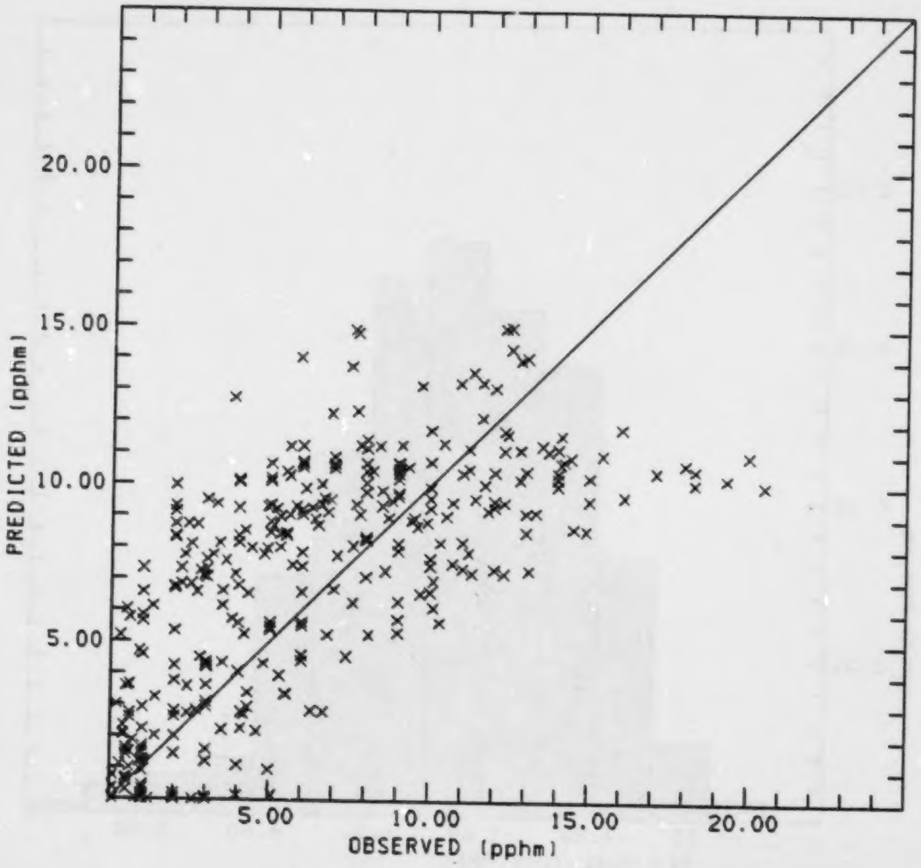
FIGURE 5-10. Concluded.

diagnostic runs 1 and 2. The predicted region-wide maximum ozone concentrations (18.2 pphm) is within 11 percent of the observed peak (20.5 pphm) and occurs approximately 45 km east of the location of the observed peak (Conshohocken). At the location of the observed peak the predicted daily maximum ozone (11.1 pphm) is only within 46 percent of the observed peak. The similarity between diagnostic runs 1 and 2 is also seen in the model performance statistics (Figure 5-11). Over all hours, diagnostic run 2 overpredicts the observed hourly ozone concentrations by about 12 percent and exhibits a gross error of about 45 percent. There is a slight improvment in the correlation coefficient in diagnostic run 2 (0.69) over diagnostic run 1 (0.68) but the difference is not significant.

PLANR Base Case

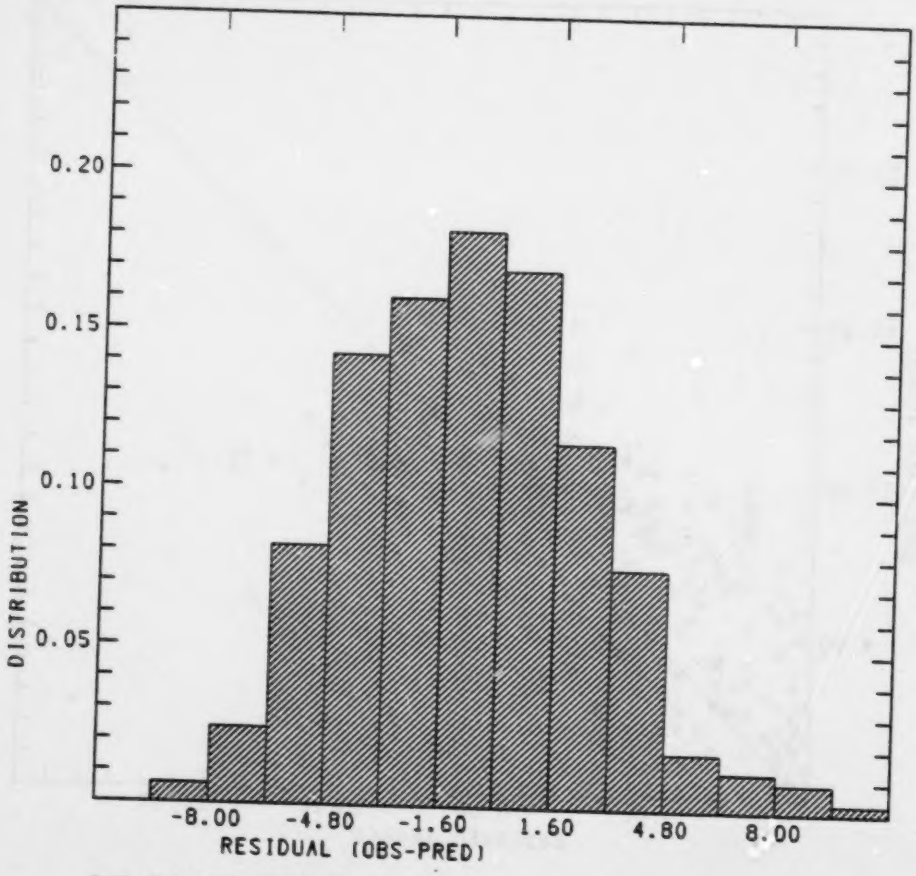
Neither of the two diagnostic runs met the model performance goal. Although the predicted region-wide maximum ozone concentrations were fairly close to the observed maximum (within 9 and 11 percent for diagnostic runs 1 and 2, respectively), the predicted peak occurs too far east (45 km) of the observed peak. In addition, the predicted daily maximum ozone at the location of the observed peak is only within 46 percent.

Even though the diagnostic simulations did not meet the performance goal, time constraints dictate that one of the simulations be selected as a PLANR UAM base case for further analysis. Thus, use of one of these simulations served as a stringent test of the effects of model performance on calculated ozone in response to emission reductions. Because diagnostic run 1 used observed data as is with no adjustments, and it has not been demonstrated that reducing wind speeds at FAA/NWS sites in the Philadelphia is justifiable, we selected diagnostic run 1 as the PLANR base case.



```
MOMENTS OF THE PROBABILITY DENSITY FUNCTION       SKILL OF PREDICTION PARAMETERS
                     OBSERVED      PREDICTED       CORRELATION COEFFICIENT OF PREDICTED
        AVERAGE      6.22966       6.98781         VERSUS OBSERVED    0.690
  STANDARD DEVIATION 4.56076       3.86320         THE BOUNDS OF THE CORRELATION AT THE
        SKEWNESS     0.64853      -0.34437         CONFIDENCE LEVEL OF 0.050 ARE
        KURTOSIS    -0.28793        -0.87080       LOW BOUND 0.629 HIGH BOUND 0.743
   OTHER MEASURES                                  RATIO OF OVER TO UNDER PREDICTIONS  1.481
        MEDIAN       5.50000       7.86000         PERCENT OF OVER PREDICTIONS
    UPPER QUARTILE   9.30000       10.00000        GREATER THAN 200 PERCENT OF THE
    LOWER QUARTILE   2.20000       3.63000         OBSERVED   22.121
     MINIMUM VALUE   0.10000       0.01000         PERCENT OF UNDER PREDICTIONS
     MAXIMUM VALUE   20.50000       15.00000       LESS THAN 50 PERCENT OF THE
                                                   OBSERVED   10.303
```

FIGURE 5-11a. Scatterplot and model performance statistics for hourly ozone concentrations in Philadelphia and deiagnostic run 2 (N = 330).



```
THE BINSIZE EQUALS  1.600

RESIDUAL ANALYSIS
          AVERAGE            -0.75822
  STANDARD DEVIATION          3.37841
          SKEWNESS            0.26279
          KURTOSIS           -0.03347
   OTHER MEASURES
           MEDIAN            -0.73000
    UPPER QUARTILE            1.41000
    LOWER QUARTILE           -3.35000
     MINIMUM VALUE           -8.93000
     MAXIMUM VALUE           10.47000
```

```
BIAS CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND -1.3011
UPPER BOUND -0.2154

STD RESIDUAL CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND 10.0878
UPPER BOUND 13.0373

THE MEASURES OF GROSS ERROR
THE ROOT MEAN SQUARE ERROR IS 3.46
THE AVERAGE ABSOLUTE ERROR IS 2.78

VARIOUS MEASURES OF RELATIVE VARIABILITY
OBSERVATION COEFFICIENT OF VARIATION
                                0.7321
RESIDUAL COEFFICIENT OF VARIATION
                                0.5423
RATIO OF RESIDUAL TO OBSERVED ST. DEV.
                                0.7408
```

FIGURE 5-11b. Residual analysis plot and model performance statistics for hourly ozone concentrations in Philadelphia and diagnostic run 2 (N = 330).

6 EVALUATION OF THE PLANR UAM APPLICATION TO PHILADELPHIA

The PLANR UAM base case simulation for Philadelphia was evaluated in two ways: (1) by comparing performance with applications of two versions of the model (UAM/CB-II and UAM/CB-IV) in which inputs were developed from a rich data base (the Philadelphia Oxidant Study, POS); and (2) by comparing the reductions in ozone concentrations calculated in the three applications in response to emission control scenarios.

COMPARISON OF MODEL PERFORMANCE

The performance of the PLANR UAM base case simulation (diagnostic run 1, discussed in Section 5) was compared with the performance of UAM simulations that used data from the Philadelphia Oxidant Study (POS). The 13 July 1979 oxidant episode in Philadelphia was used for all simulations. Routine and special surface meteorological data were available from 16 sites and surface air quality data were available from over 21 sites in the Phildelphia modeling domain (see Figure 5-2). However, because the POS was not in full operation until 18 July, no special upper-air soundings were available for 13 July 1979.

Meteorological data were developed for input to the UAM(CB-II); many diagnostic simulations were completed before a satisfactory base case was obtained (Haney and Braverman, 1985). The final base case was used in our comparison and is referred to here as UAM(CB-II). The same meteorological inputs developed from the POS data for the UAM(CB-II) were also used for the UAM(CB-IV) application that is compared here; this application is referred to as POS UAM. In the following paragraphs we briefly discuss how the modeling inputs were prepared from the POS data for the UAM(CB-II) and POS UAM; the input preparation is discussed in full by Haney and Braverman (1985). Note that the CB-IV emission inputs developed in this study differed in quantity and composition from the CB-II emissions developed previously.

Development of Inputs Using a Rich Data Base (the Philadelphia Oxidant Study)

The development of inputs for the data-intensive application of the UAM to Philadelphia required extensive data analysis and many diagnostic simulations (Haney and Braverman, 1985). Wind data were examined and questionable observations were deleted from the analysis. Surface wind data were then interpolated to create the

UAM layer 1 wind field. The winds in the top layer (layer 4 in both the UAM(CB-II) and POS UAM) were based on upper-air soundings from Dulles and JFK airports and were assumed to be constant. Following recommendations from the EPA, wind fields in the layers between layer 1 and layer 4 were obtained by linear interpolation between the wind vectors in layers 1 and 4.

A very elaborate scheme for creating mixing height fields for Philadelphia was developed to account for the urban heat island effect. As in the PLANR UAM inputs for Philadelphia, daytime mixing heights were based on the upper-air soundings at JFK and Dulles airports. At night and early morning (before 0700 EST) the nighttime minimum diffusion break was assumed to be 250 m AGL over urban areas (approximately the stipled area in Figure 4-2) and 100 m AGL over rural areas. The urban and rural mixing heights were forced to match by 0900 EST.

The UAM(CB-II) and POS UAM used the same initial concentrations (AIRQUAL) and boundary conditions (BOUNDARY) in the two layers above the mixing height (layers 3 and 4), the same boundary conditions (except for the southwest boundary) in the two layers below the mixing height, and the same concentrations above the region top (TOPCONC). These concentrations were as follows: 3 ppb NO_x; 80 ppb O_3; 58 ppbC VOC; and 200 ppb CO.

Initial concentrations in the lowest UAM layer (layer 1) were obtained by interpolating the two-hour (2300 12 July to 0100 13 July) average concentrations from the dense measurement network (see Figure 5-2). Initial concentrations in layer 2 were obtained by linear interpolation between the values in layer 1 and layer 3. Boundary conditions for the southwest boundary below the mixing height were based on measurements.

Gridded emission inventories for minor and elevated point sources and areas sources were prepared for the UAM(CB-II) by Engineering Science, Inc. in 1981 for the EPA (EPA, 1982). The POS UAM used the same emission inventory used in the PLANR UAM (see Figures 4-5 and 4-6). (The differences between the emissions inventories for UAM(CB-II) and UAM(CB-IV) (PLANR UAM and POS UAM) are shown in Table 4-4.)

The UAM(CB-II) and POS UAM simulations provide one of the first opportunities for a comparison of the CB-II and CB-IV versions of the UAM. However, differences in emissions (see Table 5-4) and in the speciation of the initial and boundary VOC concentrations complicate the comparison of the CB-II and CB-IV versions of the UAM. Other comparisons of the CB-II and CB-IV versions of the UAM—for applications to New York (Morris et al., 1989a) and St. Louis (Section 3 of this report)—were complicated by the fact that different meteorological and air quality inputs were used in each model version. In the following paragaphs we discuss the performance of the POS UAM and then compare the performance of the PLANR UAM, POS UAM, and UAM(CB-II). The performance of the UAM(CB-II) is discussed by Haney and Braverman (1985).

POS UAM Performance

The daily maximum ozone concentrations predicted by the POS UAM are shown in Figure 6-1. Time series of predicted ozone, NO, NO_2, and CO concentrations are shown in Appendix G; the predicted hourly ozone concentrations are shown in Appendix H. As seen in Figure 6-1, the region-wide maximum ozone concentration predicted by the POS UAM (23.6 pphm) is within 15 percent of the observed peak (20.5 pphm) and occurs approximately 28 km northeast of the location of the observed peak. At the location of the peak observation, the POS UAM predicts the observed peak to within 14 percent (17.7 pphm).

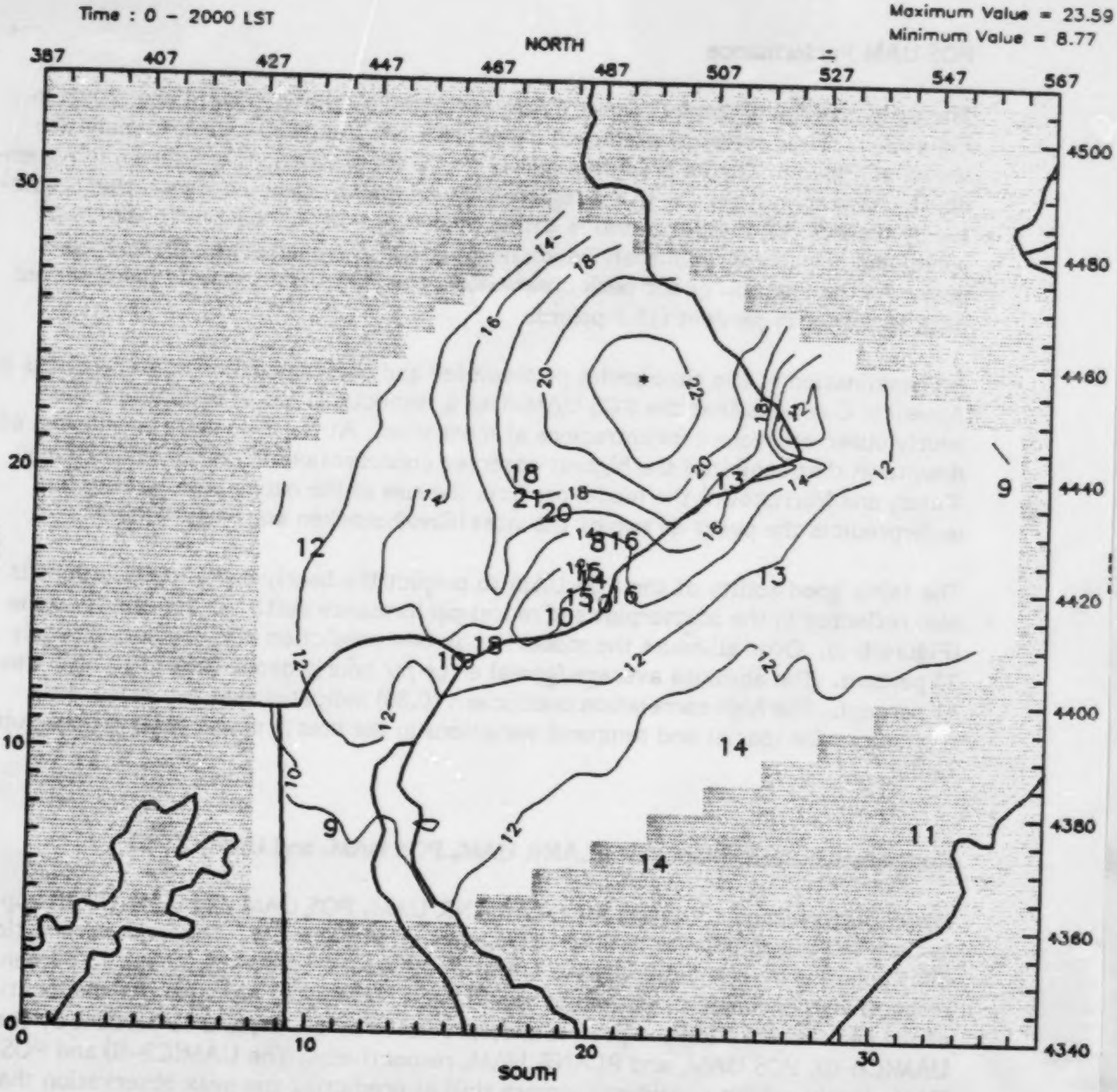
An examination of the time series of predicted and observed ozone concentrations in Appendix G reveals that the POS UAM does a respectable job of replicating the hourly observed ozone concentrations at most sites. At the three sites northwest of downtown that exhibited the highest observed concenrations (Conshohocken, Roxy Water, and Norristown) the model predicts the rise in the ozone observations but underpredicts the peaks at two of the sites (Conshohocken and Roxy Water).

The fairly good ability of the POS UAM to predict the hourly ozone observations is also reflected in the scatterplot and model performance statistics for hourly ozone (Figure 6-2). Over all hours the model has an overprediction bias of approximately 23 percent. The absolute average (gross) error for hourly ozone concentrations was 41 percent. The high correlation coefficient (0.80) indicates that the POS UAM reproduces the spatial and temporal variations in the hourly ozone observations quite well.

Comparative Performance of PLANR UAM, POS UAM, and UAM(CB-II)

Model performance statistics for the PLANR UAM, POS UAM and UAM(CB-II) applications to Philadelphia on 13 July 1979 are given in Table 6-1. The peak observation (20.5 pphm) is overpredicted by the UAM(CB-II) and POS UAM by 30 and 15 percent, respectively, and underpredicted by the PLANR UAM by 15 percent. At the location of the peak observation the peak is underpredicted by 10, 14, and 46 percent by the UAM(CB-II), POS UAM, and PLANR UAM, respectively. The UAM(CB-II) and POS UAM clearly exhibit considerably more skill at predicting the peak observation than does the PLANR UAM.

The UAM(CB-II) and POS UAM also show more skill in predicting the daily maximum ozone concentrations at the 19 ozone monitors; their bias and gross error are approximately 3 and 0.8 times lower, respectively, than the bias and gross error for the PLANR UAM. Although there are subtle differences in the performance statistics of the UAM(CB-II) and POS UAM, the differences are not statistically significant.


Time : 0 - 2000 LST
Maximum Value = 23.59
Minimum Value = 8.77
NORTH
387
407
427
447
467
487
507
527
547
567
WEST
30
20
10
0
4500
4480
4460
4440
4420
4400
4380
4360
4340
SOUTH
0
10
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14
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16
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13
15
14
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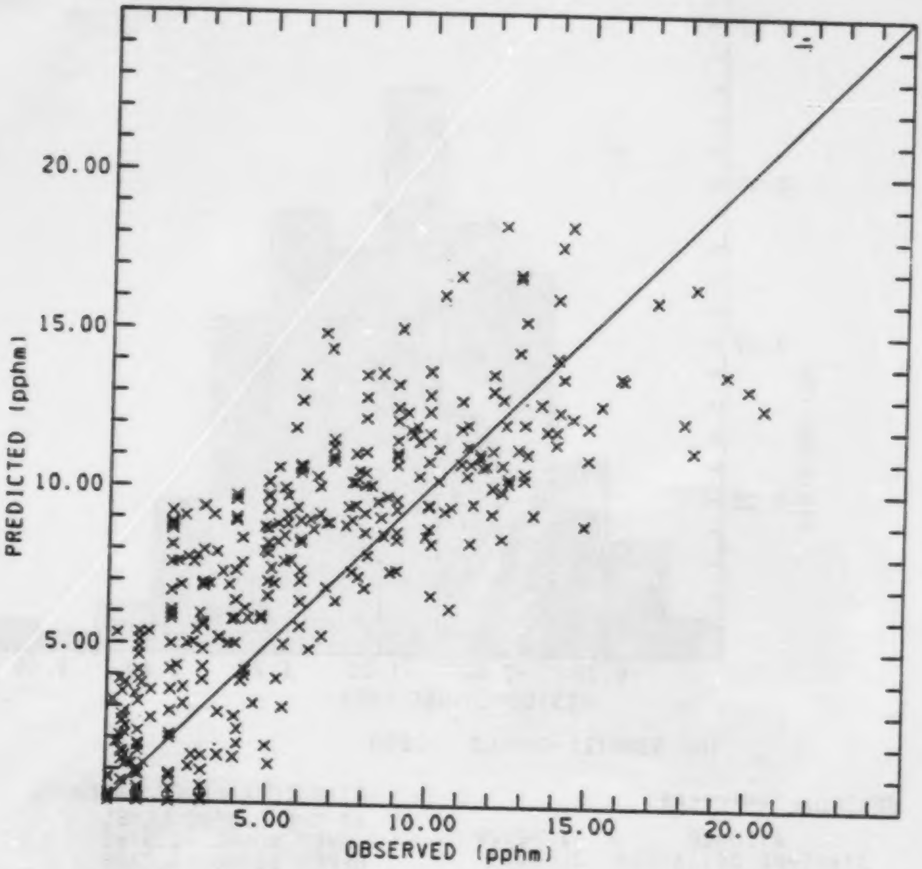
12

FIGURE 6-1. Predicted maximum daily ozone concentrations (pphm) for the POS UAM with superimposed daily maximum observations.



```
MOMENTS OF THE PROBABILITY DENSITY FUNCTION
                       OBSERVED         PREDICTED
           AVERAGE      6.22966          7.63786
STANDARD DEVIATION      4.56076          4.27899
          SKEWNESS      0.64853         -0.07555
          KURTOSIS     -0.28793           -0.71528
   OTHER MEASURES
            MEDIAN      5.50000          8.34000
    UPPER QUARTILE      9.30000         10.71000
    LOWER QUARTILE      2.20000          4.02000
     MINIMUM VALUE      0.10000          0.01000
     MAXIMUM VALUE     20.50000           18.34000
```

```
SKILL OF PREDICTION PARAMETERS
CORRELATION COEFFICIENT OF PREDICTED
VERSUS OBSERVED   0.801
THE BOUNDS OF THE CORRELATION AT THE
CONFIDENCE LEVEL OF 0.050 ARE
LOW BOUND 0.759 HIGH BOUND 0.837
RATIO OF OVER TO UNDER PREDICTIONS  2.056
PERCENT OF OVER PREDICTIONS
GREATER THAN 200 PERCENT OF THE
OBSERVED   22.727
PERCENT OF UNDER PREDICTIONS
LESS THAN 50 PERCENT OF THE
OBSERVED   8.182
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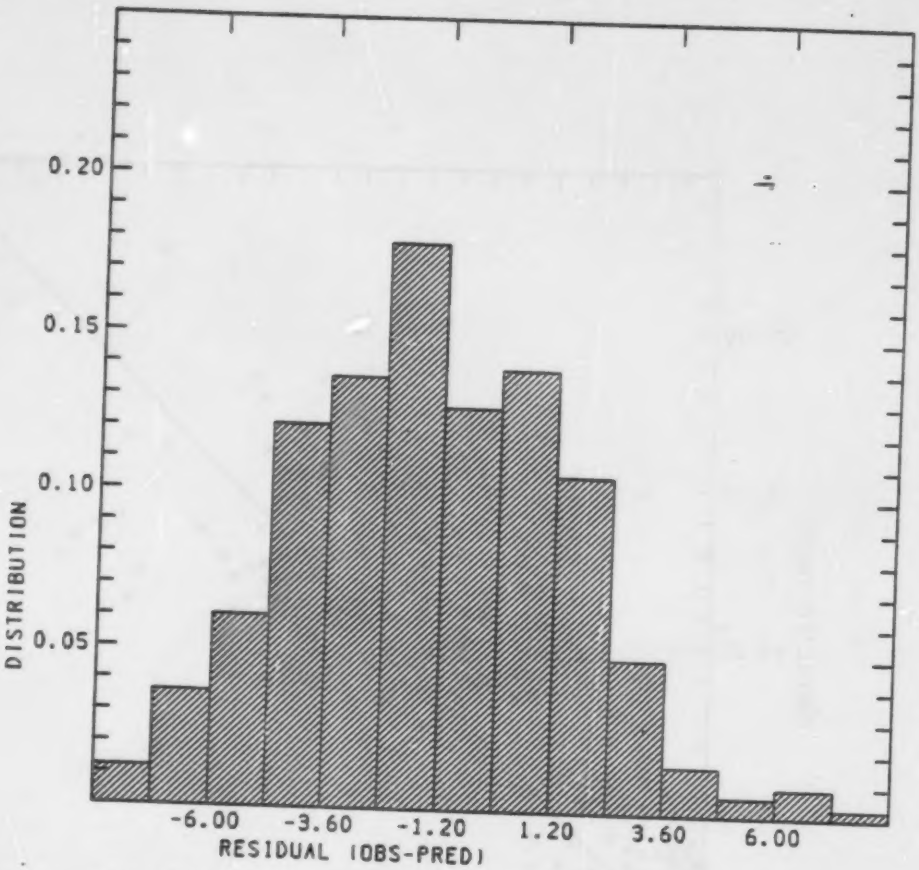
FIGURE 6-2a. Scatterplot and model performance statistics for hourly ozone concentrations in Philadelphia and POS UAM (N=330).



```
THE BINSIZE EQUALS  1.200

RESIDUAL ANALYSIS                            BIAS CONFIDENCE INTERVAL
        AVERAGE           -1.40829           AT THE 0.0500 LEVEL
  STANDARD DEVIATION      2.80004            LOWER BOUND -1.9763
        SKEWNESS          0.22466            UPPER BOUND -0.8403
        KURTOSIS          -0.00769
   OTHER MEASURES                            STD RESIDUAL CONFIDENCE INTERVAL
        MEDIAN            -1.56000           AT THE 0.0500 LEVEL
    UPPER QUARTILE        0.60000            LOWER BOUND 6.9295
    LOWER QUARTILE        -3.44000           UPPER BOUND 8.9555
     MINIMUM VALUE        -8.18000
     MAXIMUM VALUE        7.83000            THE MEASURES OF GROSS ERROR
                                             THE ROOT MEAN SQUARE ERROR IS 3.13
                                             THE AVERAGE ABSOLUTE ERROR IS 2.54

                                             VARIOUS MEASURES OF RELATIVE VARIABILITY
                                             OBSERVATION COEFFICIENT OF VARIATION
                                                                           0.7321
                                             RESIDUAL COEFFICIENT OF VARIATION
                                                                           0.4495
                                             RATIO OF RESIDUAL TO OBSERVED ST. DEV.
                                                                           0.6139
```

FIGURE 6-2b. Residual analysis plot and model performance statistics for hourly ozone concentrations in Philadelphia and POS UAM (N=330).

TABLE 6-1. Comparison of performance statistics for the UAM(CB-II), POS UAM, and PLANR UAM applications to Philadelphia for 13 July 1979.

Performance Measure	UAM (CB-II)	POS UAM	PLANR UAM
Hourly Ozone Concentrations (matched by time and location)			
Number of pairs	N/A	330	330
Average observed (pphm)	N/A	6.23	6.23
Average predicted (pphm)	N/A	7.64	7.03
Bias (pphm)	N/A	-1.41	-0.80
Average percent difference	N/A	23	13
Average absolute (gross) error (pphm)	N/A	2.54	2.82
Gross error percent difference	N/A	41	45
Correlation coefficient	N/A	0.80	0.68
Daily Maximum Ozone Concentration (matched by location but not time)			
Number of pairs	19	19	19
Average observed (pphm)	13.90	13.90	13.90
Average predicted (pphm)	14.90	13.21	11.75
Bias (pphm)	-1.00	0.69	2.15
Average percent difference	7	5	16
Average absolute (gross) error (pphm)	2.02	2.21	3.60
Gross error percent difference	15	16	26
Correlation coefficient	0.73	0.72	-0.10
Peak Ozone Concentration			
Peak observed (pphm)	20.5	20.5	20.5
Unmatched by time or location:			
Predicted region-wide maximum (pphm)	26.6	23.6	18.7
Ratio of prediction to observation	1.30	1.15	0.91
Matched by location but not time:			
Predicted maximum (pphm)	18.5	17.7	11.1
Ratio of prediction to observation	0.90	0.86	0.54
Hours difference in prediction to observation	+2	0	0

Discussion

The seemingly "good" performance of the POS UAM (and UAM(CB-II)) compared to the "poor" model performance of the PLANR UAM is due to differences in the following inputs:

Layer Structure: The POS UAM used four vertical layers, two below and two above the diffusion break, whereas the PLANR UAM used five vertical layers, two below and three above the diffusion break.

Wind Fields (WIND): The POS UAM wind field was generated using meteorological data from 16 surface and two upper-air meteorological observations sites. The data were extensively screened and the wind field was created after several iterations of data manipulation, variations of interpolation techniques, and diagnostic simulations. The PLANR UAM wind field was generated from just the routine data (11 surface and two upper-air sites). The routine data were used in the PLANR UAM wind preprocessor without any adjustments.

Mixing Heights (DIFFBREAK): The POS UAM used nighttime and morning mixing heights that neglected the presence of the urban heat island. The nocturnal mixing height was 250 m AGL over the urban areas and 100 m AGL over the rural areas. The daily maximum mixing height used in the PLANR UAM (1775 m AGL) was approximately 16 percent (250 m) higher than that used in the POS UAM (1525 m AGL). At night, the PLANR UAM used the same diffusion break value as the POS UAM in urban regions (250 m AGL), but over rural regions the PLANR UAM diffusion break (250 m AGL) was 2.5 times the value used in POS UAM (100 m AGL).

Other Meteorological Inputs: Temperature gradients, water vapor concentrations (METSCALERS), and surface temperatures (TEMPERATUR) were also different in the POS and PLANR UAM.

Initial Concentrations (AIRQUAL): The initial concentrations used in the POS and PLANR UAM are quite different. Because there were no routine VOC measurements, "clean" values were used in the PLANR UAM application to Philadelphia. In addition, since no routine air quality measurements aloft were available, "clean" values were used for NO_x, ozone, and VOC for initial concentrations for the PLANR UAM in layers above the DIFFBREAK (250 m AGL). In contrast, considerable analysis of the extensive POS data base went into the development of the initial condition concentrations below and above the DIFFBREAK for the POS UAM. In total, the initial VOC and ozone concentrations were approximately 4 and 2 times greater in the POS UAM than the values used in the PLANR UAM. Initial NO_x concentrations were about the same; initial NO_x was about 15 percent lower in POS UAM than in PLANR UAM.

Boundary Conditions Aloft (TOPCONC): Boundary conditions above the region top were much higher in POS UAM than in PLANR UAM. Assumed concentrations of NO_x, VOC, and ozone were 2 to 3 times higher in the POS UAM than in the PLANR UAM.

The primary differences between the POS and PLANR UAM simulations can be divided into two catgories: meteorology (winds, mixing heights, temperatures, and metscalers) and air quality (initial and boundary conditions). It is difficult ascertain whether the differences between the POS and PLANR UAM are primarily due to meteorology or air quality inputs. Thus a sensitivity simulation was performed that used the PLANR UAM meteorological inputs (WINDS, DIFFBREAK, METSCALERS, and TEMPERATUR) and the POS UAM air quality inputs (AIRQUAL, BOUNDARY, and TOPCONC). The results of the meteorology sensivity test are displayed in Appendix I.

As seen in Appendix I, the sensitivity test produces results that are very similar to the PLANR UAM; there is a very slight improvement in model performance. The predicted region-wide maximum ozone in the sensitivity test is within 14 percent, compared to 19 percent for the PLANR UAM. However, the predicted elevated ozone cloud in the meteorological sensitivity test is still too far to the east. Thus the reason for the "good" model performance of the POS UAM and UAM(CB-II) is due to the meteorological inputs. In order to obtain better model performance in the PLANR UAM, the wind fields would have to be altered so that the elevated ozone cloud is retained north of downtown.

CORRECTIONS FOR MODEL BIAS IN CALCULATIONS OF OZONE CONCENTRATIONS IN RESPONSE TO EMISSION CONTROL STRATEGIES

As was done for the St. Louis analysis, we examined three different techniques for accounting for model bias when using the model to demonstrate attainment of the ozone NAAQS: the uncorrected bias approach, the decrement approach, and the percentage approach (see Section 4 for explanation).

The POS UAM, PLANR UAM, and UAM(CB-II) were exercised for uniform (across the board) VOC emission control scenarios. In the POS UAM simulations the VOC initial and boundary conditions in excess of background (25 ppbC) were reduced the same percentage as the VOC emissions in these control scenarios. However, because the PLANR UAM used background initial and boundary VOC concentrations, the same initial and boundary conditions were used for all of the PLANR UAM emission control simulations. The UAM(CB-II) VOC emission control scenarios also used the same VOC initial and boundary conditions (Haney and Braverman, 1985).

The region-wide maximum ozone concentration calculated in the VOC emission control scenarios are given in Table 6-2. When overprediction (POS UAM and UAM(CB-II)) or underprediction (PLANR UAM) of the observed peak is not accounted for (the

TABLE 6-2. Predicted region-wide maximum ozone concentrations for the POS UAM, PLANR UAM, and UAM(CB-II) for VOC emission reduction scenarios.

Percent VOC Emission Reduction	Region-wide Maximum Ozone Concentration (pphm)		
	POS UAM	PLANR UAM	UAM(CB-II)*
0	23.6	18.7	26.6
25	N/A	N/A	20.6
50	N/A	N/A	14.7
60	13.9	12.2	N/A
75	N/A	N/A	12.4
90	10.6	10.8	N/A

* From Haney and Braverman, 1985.

uncorrected bias approach), it is estimated from the data in Table 6-2 that the reductions of VOC emissions required to reduce ozone concentrations to below the NAAQS (12 pphm) are 77 percent for POS UAM, 79 percent for UAM(CB-II), and 64 percent for PLANR UAM. This result is as expected when model bias is not corrected: the higher the predicted region-wide maximum ozone concentration, the steeper the VOC emission reductions that are needed to reduce the peak ozone concentration to the NAAQS.

Using the decrement approach, the POS UAM results yield a 54 percent reduction in VOC emissions, whereas the PLANR UAM results mean that over 90 percent of the VOC emissions would have to be eliminated for ozone attainment. The UAM(CB-II) estimates that a 36 percent reduction in VOC emissions is needed. The extra emission reduction required by the PLANR UAM, compared to the POS UAM, is not surprising in view of the underprediction of the peak observations by the PLANR UAM and overprediction by the POS UAM. Also, in the PLANR UAM more of the predicted peak ozone concentration is due to the irreducible background. The difference in VOC reductions for UAM(CB-II) and POS UAM is somewhat surprising, however, since the modeling inputs were essentially the same. Furthermore, in the POS UAM initial and boundary conditions were also reduced in the emission reduction scenarios, whereas they were not in the UAM(CB-II). The only explanations are (1) the peak observation predicted by the UAM(CB-II) (30 percent) is higher than that of POS UAM (15 percent); (2) different chemical mechanisms were used; and (3) the emissions were different.

Using the percentage approach, POS UAM, PLANR UAM, and UAM(CB-II) results yield respectively 61, 87, and 46 percent reductions in VOC emissions. The differences between the POS UAM and PLANR UAM reductions are related to the over- and underprediction of the observed peak and the fact that urban emissions have less influence on the PLANR UAM ozone peak because of the model's poor performance in locating the peak. Since the modeling inputs for the POS UAM and UAM(CB-II) are very similar, the differences in the levels of VOC emission reductions for the two models is more difficult to explain. Because of the major differences in the model inputs (the initial and boundary conditions) for POS UAM and UAM(CB-II) VOC emission control scenarios, we would expect the POS UAM to calculate that less VOC emission reductions are needed for attainment than the UAM(CB-II), yet the opposite is actually true. The differences between the POS UAM and UAM(CB-II) VOC reduction requirements for ozone attainment are most likely related to the higher overprediction of the observed peak in the UAM(CB-II) and the fact that the CB-IV chemical mechanism tends to estimate larger VOC emission reductions to reduce ozone concentrations than does CB-II.

The VOC emissions reductions needed to reduce the peak ozone concentration to 12 pphm, as calculated by the POS UAM, PLANR UAM, and UAM(CB-II) and using the uncorrected, decrement, and percentage approaches to model bias, are given in Table 6-3. When model bias is accounted for, PLANR UAM always calculates larger VOC

TABLE 6-3. Percent VOC emission reduction required to reduce the calculated region-wide maximum ozone concentration to 12 pphm in Philadelphia based on the POS UAM, PLANR UAM, and UAM(CB-II) applications and different approaches for correcting model bias.

Approach	POS UAM	PLANR UAM	UAM(CB-II)
Uncorrected Bias	77	64	79
Decrement	54	>90	36
Percentage	61	87	46

emission reductions to reach attainment than does the POS UAM, whereas the POS UAM always calculates larger emission reduction requirements than does the UAM(CB-II). The difference in results for the PLANR UAM and POS UAM is related to the difference in wind fields. The POS UAM wind field recirculates the urban emissions from Phildelphia, resulting in a higher predicted ozone peak near downtown. The PLANR UAM peak occurs further downwind of downtown, where the emissions are more diffuse and more of the peak is due to background (initial and boundary) conditions. In addition, the VOC emission reduction scenarios for the POS UAM also include significant reductions in the initial VOC concentrations, approximately 35 and 52 percent reductions for the 60 and 90 percent VOC emission control scenarios respectively. However, because "clean" concentrations were used for the initial conditions in the PLANR UAM, the initial conditions for PLANR UAM were not reduced in the VOC emission control scenarios. As noted above, the differences in the VOC emission reductions for ozone attainment calculated by the POS UAM and UAM(CB-II) are related to the higher predicted peak in the UAM(CB-II) and the chemical mechanisms used.

7 SUMMARY AND RECOMMENDATIONS

This study evaluated a simpler approach for the application of the Urban Airshed Model, the Practice for Low-Cost Airshed-Ppplication for Nonattainment Regions (PLANR). In this approach only routinely available data are used and a limited number of diagnostic simulations are performed to establish a base case. The PLANR UAM approach was used to simulate two ozone episodes: 13 July 1976 in St. Louis and 13 July 1979 in Philadelphia. Extensive field measurement programs conducted during these episodes provided rich data bases for evaluating the PLANR UAM performance—the Regional Air Pollution Study (RAPS) in St. Louis and the Philadelphia Oxidant Study (POS) in Philadelphia. The PLANR UAM simulations were evaluated several different ways: (1) the predictions were compared with observations from the rich data base; (2) the model performance was compared with that of the UAM (CB-II) and UAM (CV-IV) in which the rich data base was used as inputs; and (3) the calculated reductions in ozone concentrations in response to VOC emission reductions were compared with those of the UAM (CB-II) and UAM (CV-IV).

ST. LOUIS TEST

The first step in any PLANR use of the UAM is the characterization of the meteorological conditions that existed during the ozone episode. For St. Louis on 13 July 1976 these conditions included the passage of a warm front through the area and a corresponding passage of a high-pressure system to the north that caused a wind shift at around noon.

For the St. Louis episode of 13 July 1976 three diagnostic simulations were necessary before the model sufficiently replicated the peak ozone observations. These diagnostic simulations differed in the interpretation and use of the routine meteorological data for input. The first diagnostic simulation used the observed upper-air sounding from a site west of St. Louis; although this site was farther away than the monitoring site to the east, it was on the same side of the warm front during the afternoon. The second diagnostic simulation used upper-air observations from the site east of St. Louis for the morning, and the soundings from the west site for the afternoon. For the third diagnostic simulation, wind observations at FAA sites were used but reduced 50 percent. During conditions typically associated with ozone episodes (low wind speeds), hourly average wind speeds may be as low as 50 percent of those reported at FAA stations.

The performance of the PLANR use of the UAM (inputs prepared from routine observations only) was compared with that of the conventional use of the UAM (inputs prepared from a rich data base). In this comparison the old version of the UAM (the UAM(CB-II) and its preprocessors) and the latest version (the UAM(CB-IV) and its preprocessors) were subjected to a comprehensive performance evaluation using observations from the extensive data in the RAPS data base. In addition, the UAM was exercised using a very simplified data base (SIMPLE UAM), i.e., using meteorological conditions from a single surface site and mixing heights from the nearest upper-air site. The results of these comparisons are as follows. In a comparison of the peak predicted and observed ozone concentrations unmatched by time or location, the UAM(CB-II) and the RAPS, PLANR, and SIMPLE UAM calculated the peak observation to within, respectively, 22, 9, 12, and 47 percent of the observed peak. Thus, the UAM(CB-IV) performed better when an extensive data base was used (RAPS UAM) than when only routinely available data were used (PLANR UAM). However, even though it used only routinely available data, the PLANR UAM (with CB-IV) performed better than the UAM (CB-II), which used the extensive data base. The use of the UAM with very simple inputs and no diagnostic simulations (SIMPLE UAM) resulted in very poor model performance.

It should be noted that the PLANR UAM's underprediction of the peak observed ozone by 12 percent may be due entirely to deficiencies in the 1976 emission inventory used. Since that time several sources of previously uninventoried hydrocarbon emissions (mobile source running loss emissions, temperature effects on evaporative emissions, previously unaccounted for VOC emissions, biogenic emissions, etc.) have been quantified that would substantially increase the predicted ozone concentrations.

The RAPS, PLANR, and SIMPLE UAM were also exercised for a series of VOC emission control scenarios to determine what effects rich versus sparse inputs have on calculated ozone reductions in reponse to VOC emission reductions. Because the maximum ozone concentrations predicted by the model did not exactly match the observed peaks, several methods of correcting model bias were also studied. When correcting for model bias, the PLANR UAM calculated 5 to 18 percent less VOC emission reductions to reach attainment of the ozone NAAQS than did the RAPS UAM; the SIMPLE UAM calculated that from -8 to over 22 percent more VOC emission reductions to reach attainment than did the RAPS UAM.

Three different methods of treating model bias were analyzed. For the RAPS UAM calculations the results of the three methods varied only 5 percentage points (78 to 53 percent VOC emissions reductions needed to achieve attainment of the ozone NAAQS). For the PLANR UAM calculations the results of the methods varied 9 points (64 to 73 percent), and for the SIMPLE UAM they varied over 26 points (74 to > 100 percent). Clearly, the RAPS and PLANR UAM are more robust tools for calculating the emission reductions needed to attain the ozone NAAQS than is the SIMPLE UAM. When UAM model performance is extremely poor, as in the SIMPLE UAM, the model should not be used for emission control strategies.

PHILADELPHIA TEST

The Philadlephia ozone episode of 13 July 1979 was characterized by hot stagnant conditions. Winds were light and appeared to advect the urban emissions south in the morning of 13 July and then north back across downtown, resulting in the high ozone exceedances measured to the northwest of downtown. The occurrence of high measured ozone concentrations in the morning indicated that there was a significant reservoir of ozone aloft.

Two diagnostic simulations were performed for Philadelphia: in one the observed data were used without adjustments, and in the other the observed surface wind speeds at FAA sites were used but reduced by 50 percent. The results of the two diagnostic runs were almost identical. The predicted peak ozone concentration was lower than the observed peak and occurred too far to the east. To obtain better model performance the wind fields would have to be subjectively altered to retain the urban emissions in the vicinity of downtown Philadelphia. Since one of the principal objectives of this study is to evaluate the utility of running the UAM with objectively prepared inputs from just routine data, the alteration of the wind fields to predict peak ozone concentrations closer to the observed peak ozone observations would not be consistent with the PLANR use of the UAM since the sites with the peak observations were not routine observations. Thus diagnostic run 1 was selected as the base case because it used the routine data with no adjustments.

The performance of the PLANR UAM application to Philadelphia was compared with the performance of the UAM when model inputs were prepared from a rich data base, the Philadelphia Oxidant Study (POS). The applications based on the POS data used the UAM(CB-II) and UAM(CB-IV), the latter referred to as POS UAM to distinguish it from the PLANR application of UAM(CB-IV). The region-wide maximum ozone concentrations calculated by the POS UAM, UAM(CB-II), and PLANR UAM were within 15, 30, and 9 percent, respectively, of the observed peak. At the location of the observed peak the PLANR UAM underpredicted the observation by 46 percent, whereas both the POS UAM and UAM(CB-II) replicated the observed peak to within 15 percent. In general, the performance of the POS UAM and UAM(CB-II) was quite good, while the PLANR UAM tended to underpredict the observed daily maximum ozone concentrations at most sites.

As in the St. Louis applications, the PLANR UAM underprediction of the highest observed ozone concentrations can be partly attributable to known sources of VOC emissions that were missing from the 1979 inventory. However, since the PLANR UAM predicts an elevated ozone cloud approximately 40 km east of the location of the highest observations, it appears that the wind field used in the PLANR UAM does not represent actual flow patterns on 13 July 1979. The PLANR UAM wind field problem was confirmed by a sensitivity simulation in which the air quality inputs (initial and boundary conditions) of the POS UAM were used as inputs; the results very similar to the PLANR UAM base case.

The PLANR UAM, POS UAM, and UAM(CB-II) were exercised for a series of VOC emission reduction scenarios designed to determine the level of VOC reductions needed to reduce the peak observation to below the NAAQS. When correcting for model bias, the PLANR UAM calculates 26 to over 36 percent more VOC emission reductions than does the POS UAM. The UAM(CB-II) calculated 15 to 18 percent less VOC emissions reductions than the POS UAM.

Differences in VOC emission reductions calculated by the PLANR and POS UAM can be attributed to the fact that the POS UAM has a recirculating wind field which resulted in urban emissions contributing most of the ozone precursors in the vicinity of the predicted peak, whereas the PLANR UAM predicted peak occurred further downwind where the initial and boundary conditions had a larger contribution to the ozone precursors.

Since the POS UAM and UAM(CB-II) used almost identical inputs, the differences in their calculations of the VOC emission reductions needed to demonstrate attainment are more difficult to explain. It appears that the VOC emission reductions calculated by UAM(CB-II) are lower because the model predicts a higher peak in the base case and because the CB-II chemical mechanism tends to calculate lower VOC emission reductions needed for attainment than does the CB-IV.

Because of the large amounts of transported pollutants known to exist in the Philadelphia region and the complex meteorological conditions (stagnation with wind shear) that existed on 13 July 1979, this episode is most likely not an appropriate choice for evaluating the PLANR use of the UAM. Extensive data bases or regional modeling studies are needed to characterize transport in the northeastern U.S. Fortunately the EPA is currently conducting such a modeling study, the Regional Oxidant Modeling for Northeast Transport (ROMNET) program, in which a regional oxidant model is used to define boundary conditions for the UAM in cities in the northeast.

RECOMMENDATIONS

The evaluation of the PLANR use of the UAM to simulate two historical episodes in St. Louis and Philadelphia was inconclusive because of known deficiences in the emission inventories used and because the model applications deviated slightly from the PLANR use of the UAM (i.e., nonroutine data had to be used for model evaluation). In the PLANR UAM application to Philadelphia routine meteorological observations were used as is for the base case, and the model exhibited rather poor performance. Because there were no routine ozone observations in St. Louis during the modeled episode, ozone observations from a special study were used (for evaluation only) to develop a PLANR UAM base case, which exhibited good model performance.

The PLANR use of the UAM needs to be tested with additional cities and ozone episodes. So far, the PLANR use of the UAM has been tested for St. Louis, Philadelphia, Atlanta, and Dallas-Fort Worth. However, St. Louis and Philadelphia were the only areas with the data needed to compare the PLANR UAM with a conventional UAM application (that is, one based on an extensive data base). The PLANR UAM also needs to be applied to more recent episodes so that more recent, higher-quality emission inventories can be used. For the PLANR approach, inputs should be developed using only routine meteorological and air quality data, and the diagnostic simulations performed to arrive at a base case should be evaluated using only the routine air quality data. Once the PLANR UAM base case is developed, special study air quality data can be used to evaluate the PLANR results. In addition, side-by-side simulations of an episode using both PLANR and conventional applications of the UAM would be desirable for evaluating PLANR results.

Of highest priority in the use of the UAM to demonstrate ozone attainment is the development of high-quality emission inventories for air quality modeling. In many past UAM modeling studies meteorological inputs were altered to get model predictions to match the observations. Because past emission inventories are known to understate the amount of VOC emissions, these alterations may have been unwarranted. Although much progress has been made over the last 10 years in the development of higher-quality emission inventories, further progress is needed before a comprehensive emission control strategy to eliminate the ozone problem can be developed.

References

Allard, D., M. Chan, C. Marlia, and E. Stephens. 1981. Philadelphia Oxidant Data Enhancement Study--Analysis and Interpretation of Measured Data. U.S. Environmental Protection Agency (EPA-450/4-81-011).

Ames, J., T. C. Myers, L. E. Reid, D. C. Whitney, S. H. Golding, S. R. Hayes, and S. D. Reynolds. 1985a. SAI Airshed Model Operations Manuals. Volume I--User's Manual. U.S. Environmental Protection Agency (EPA-600/8-85-007a).

Ames, J., S. R. Hayes, T. C. Myers, and D. C. Whitney. 1985b. SAI Airshed Model Operations Manuals. Volume II--System's Manual. U.S. Environmental Protection Agency (EPA-600/8-85-007b).

Bass, A. M., L. C. Glasgow, C. Miller, J. P. Jesson, and D. L. Filken. 1980. Planet Space Sci., 28:675.

Boris, J. P., and D. L. Book. 1973. Flux-corrected transport: I. SHASTA, a fluid transport algorithm that works. J. Comp. Phys., 11:38-69.

Burton, C. S. 1988. Comments on "Ozone Air Quality Models." J. Air Pollut. Control Assoc., 38(9):1119-1128.

Chameides, W. L., R. W. Lindsay, J. Richardson, and C. S. Kiang. 1988. The role of biogenic hydrocarbons in urban photochemical smog: Atlanta as a case study. Science, 241:1473-1475.

Chock, D. P., and A. M. Dunker. 1983. A comparison of numerical methods for solving the advection equation. Atmos. Environ., 17:11-24.

Chock, D. P. 1985. A comparison of numerical methods for solving the advection equation--II. Atmos. Environ., 19:571-586.

Cole, H. S., D. E. Layland, G. K. Moss, and C. F. Newberry. 1983. The St. Louis Ozone Modeling Project. U.S. Environmental Protection Agency (EPA-450/4-83-019).

Douglas, S., and R. Kessler. 1988. "User's Guide to the Diagnostic Wind Model. Version 1.0." Systems Applications, Inc., San Rafael, California.

EPA. 1982. Emissions Inventories for Urban Airshed Model Application in the Philadelphia AQCR. U.S. Environmental Protection Agency (EPA-450/4-82-005).

EPA. 1986. Guideline on Air Quality Models (Revised). U.S. Environmental Protection Agency (EPA-450/2-78-027R).

Gery, M. W., G. Z. Whitten, and J. P. Killus. 1988. "Development and Testing of the CBM-IV for Urban and Regional Modeling." Systems Applications, Inc., San Rafael, California (SYSAPP-88/002).

Godden, D., and F. Lurmann. 1983. "Development of the PLMSTAR Model and Its Application to Ozone Episode Conditions in the South Coast Air Basin." Environmental Research & Technology, Inc., Westlake Village, California (ERT P-A702-200).

Haney, J. L., and T. N. Braverman. 1985. Evaluation and Application of the Urban Airshed Model in the Philadelphia Air Quality Control Region. U.S. Environmental Protection Agency (EPA-450/4-85-993).

Haney, J. L., and C. S. Burton. 1988. "UAM-CMB-IV-Calculated Effects of Emission Reductions on Ozone Levels in the Philadelphia Metropolitan Area." Systems Applications, Inc., San Rafael, California (SYSAPP-88/117).

Haney, J. L., D. R. Souten, T. W. Tesche, L. R. Chinkin, H. Hogo, and M. C. Dudik. 1986. "Evaluation and Applications of the PARIS Photochemical Model in the South Central Coast Air Basin." Volume I. Systems Applications, Inc., San Rafael, California (SYSAPP-86/065).

Hogo, H., L. A. Mahoney, and M. A. Yocke. 1988. "Draft Air Quality Management Plan 1988 Revision. Draft Appendix V-R. Urban Airshed Model Performance Evaluation for 5-7 June 1985." Systems Applications, Inc., San Rafael, California (SYSAPP-88/138).

Layland, D. E., and H. S. Cole. 1983. A Review of Recent Applications of the SAI Urban Airshed Model. U.S. Environmental Protection Agency (EPA-450/4-84-004).

Morris, R. E., M. W. Gery, M. K. Liu, G. E. Moore, C. Daly, and S. M. Greenfield. 1989d. "Sensitivity of a Regional Oxidant Model to Variations in Climate Parameters. Volume I: Results." Systems Applications, Inc., San Rafael, California (SYSAPP-89/014a).

Morris, R. E., R. C. Kessler, S. G. Douglas, K. R. Styles, and G. E. Moore. 1988. "Rocky Mountain Acid Deposition Model Assessment Acid Rain Mountain Mesoscale Model (ARM3)." Systems Applications, Inc., San Rafael, California (SYSAPP-88/152).

Morris, R. E., T. C. Myers, E. L. Carr, and M. C. Causley. 1989c. "Urban Airshed Model Study of Five Cities. Demonstration of Low-Cost Application of the Model to the City of Atlanta and the Dallas-Fort Worth Metroplex Regions." Systems Applications, Inc., San Rafael, California (SYSAPP-89/122).

Morris, R. E., T. C. Myers, M. C. Causley, and L. Gardner. 1989b. "Low-Cost Application of the Urban Airshed Model to Atlanta and Evaluation of the Effects of Biogenic Emissions on Emission Control Strategies." Systems Applications, Inc., San Rafael, California.

Morris, R. E., T. C. Myers, H. Hogo, L. R. Chinkin, L. A. Gardner, and R. G. Johnson. 1989a. "A Low-Cost Application of the Urban Airshed Model to the New York Metropolitan Area and the City of St. Louis." Systems Applications, Inc., San Rafael, California (SYSAPP-89/038).

O'Brien, J. J. 1970. A note on the vertical structure of the eddy exchange coefficient in the planetary boundary layer. J. Atmos. Sci., 27:1213-1215.

OTA. 1988a. "Urban Ozone and the Clean Air Act: Problems and Proposals for Change." Office of Technology Assessment, Washington, D.C.

OTA. 1988b. "Ozone and the Clean Air Act: Summary of OTA Workshop with State and Local Air Pollution Control Agency Officials." Office of Technology Assessment, Washington, D.C.

OTA. 1988c. "Ozone and the Clean Air Act: A Summary of OTA Workshops on Congressional Options to Address Nonattainment of the Ozone Standard." Office of Technology Assessment, Washington, D.C.

Rao, S. T. 1987. Application of the Urban Airshed Model to the New York Metropolitan Area. U.S. Environmental Protection Agency (EPA-450/4-87-011).

Ross, D. G., and I. Smith. 1986. "Diagnostic Wind Field Modeling for Complex Terrain—Testing and Evaluation." Centre for Applied Mathematical Modeling, Chisholm Institute of Technology (CAMM Report No. 5/86).

SAI. 1989. "User's Manual for Preparing Emission Files for Use in the Urban Airshed Model." Systems Applications, Inc., San Rafael, California (SYSAPP-89/114).

Schere, K. L. 1983. An evaluation of several numerical advection schemes. Atmos. Environ., 17:1897-1907.

Schere, K. L., and K. L. Demerjian. 1977. Calculation of Selected Photolytic Rate Constants over a Diurnal Range. A Computer Algorithm. U.S. Environmental Protection Agency (EPA-600/4-77-015).

Schere, K. L., and J. H. Shreffler. 1982. Final Evaluation of Urban-Scale Photochemical Air Quality Simulation Models. U.S. Environmental Protection Agency (EPA-600/3-82-094).

Science. 1988. Rural and urban ozone. Editorial in Science, 241(4873):1569.

Seinfeld, J. H. 1988a. Ozone air quality models. A critical review. J. Air Pollut. Control Assoc., 38(5):616.

Seinfeld, J. H. 1988b. Closing remarks. J. Air Pollut. Control Assoc., 38(8):1136-1137.

Smolarkiewicz, P. K. 1983. A simple positive definite advection scheme with small implicit diffusion. Monthly Weather Review, 111:479-486.

Whitten, G. Z., J. P. Killus, and H. Hogo. 1980. Modeling of Simulated Photochemical Smog with Kinetic Mechanisms. Volume 1. U.S. Environmental Protection Agency (EPA-600/3-80-028a).

Whitten, G. Z., T. C. Meyers, C. Daly, L. R. Chinkin, S. D. Reynolds, N. M. Yonkow, and B. Austin. 1985. "Application of the Urban Airshed Model to Kern County." Systems Applications, Inc., San Rafael, California (SYSAPP-85/200).

Yamartino, R. J., and J. S. Scire. 1984. "ADOM/TADAP Model Development Program. Volume 3. The Transport and Diffusion Modules." Environmental Research & Technology, Inc., Concord, Massachusetts (P-B980-210).

Yocke, M. A., R. E. Morris, H. Hogo, L. R. Chinkin, and L. A. Mahoney. 1985. "Analysis of the Air Quality Impacts of the San Miguel Project. Volume I." Systems Applications, Inc., San Rafael, California (SYSAPP-85/127).

Zalesak, S. T. 1979. Fully multi-dimensional flux-corrected transport algorithms for fluids. J. Comput. Phys., 31:335-362.

Appendix A

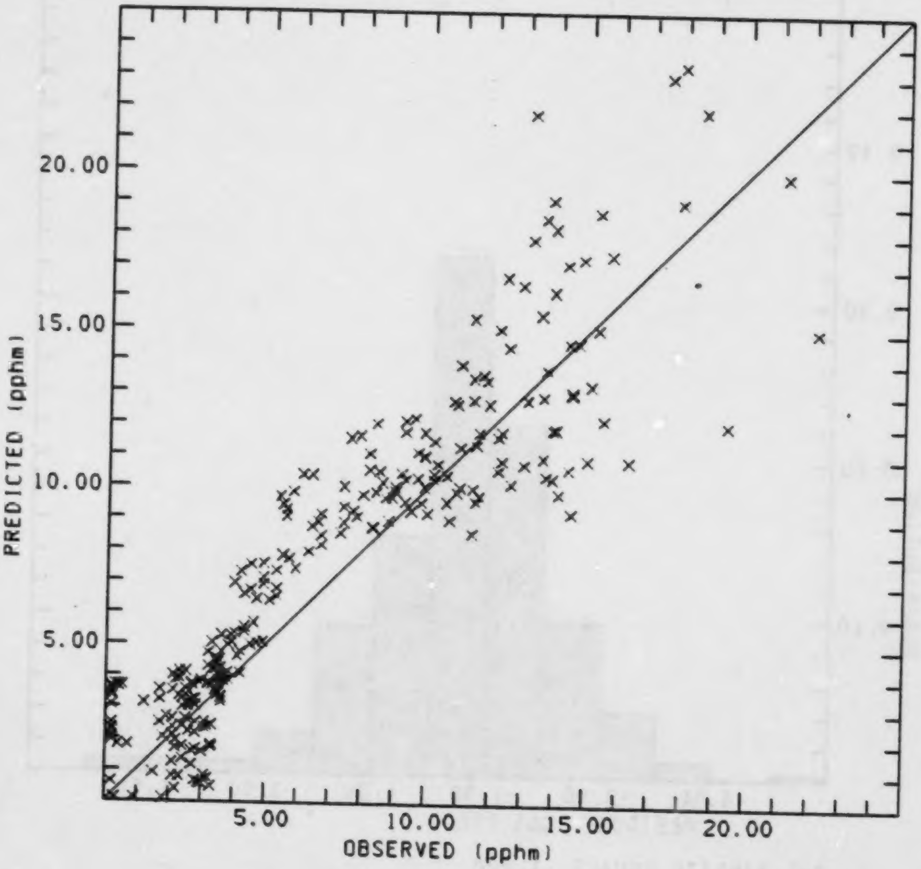
MODEL PERFORMANCE STATISTICS FOR HOURLY AND DAILY MAXIMUM OZONE CONCENTRATIONS FOR THE RAPS, PLANR, AND SIMPLE UAM APPLICATIONS TO ST. LOUIS

Appendix

Scatterplots, residual analysis plots, and model performance statistics for:

A-1	RAPS UAM hourly ozone concentrations
A-2	RAPS UAM daily maximum ozone concentrations
A-3	PLANR UAM hourly ozone concentrations
A-4	PLANR UAM daily maximum ozone concentration
A-5	SIMPLE UAM hourly ozone concentrations
A-6	SIMPLE UAM daily maximum ozone concentrations

```
VARIABLE...OZONE
BEGINNING DATE...8/8/80
ENDING DATE...8/8/80
OBSERVATION SOURCE...OZONE
OBSERVATION ANALYSIS...AIRS DATA
THE PREDICTION ALGORITHM...UAM(CB-IV) OZONE
AVERAGING TIME...ALL HOURS
STRATITFYING VARIABLE...AIRS DATA SITES
SAMPLE SIZE...265
```

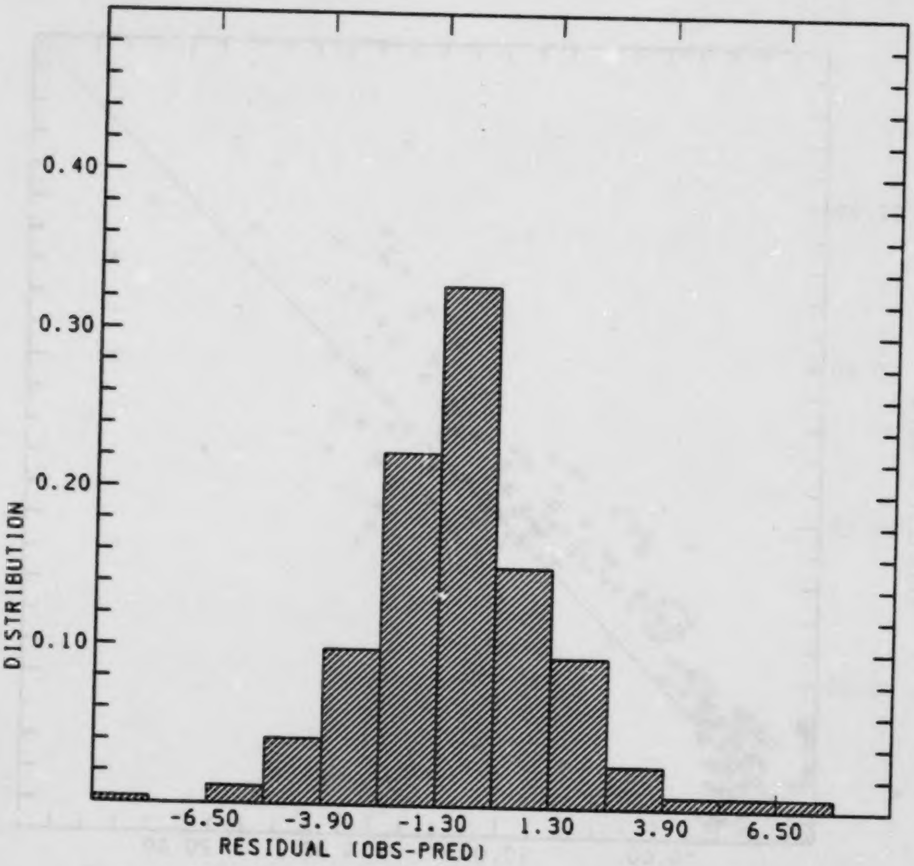


```
MOMENTS OF THE PROBABILITY DENSITY FUNCTION
                       OBSERVED       PREDICTED
        AVERAGE        6.77843        7.51675
  STANDARD DEVIATION   4.85895        4.99583
        SKEWNESS       0.68694        0.69536
        KURTOSIS       -0.47257        -0.01638
   OTHER MEASURES
        MEDIAN         4.90000        6.79000
    UPPER QUARTILE     10.60000        10.57000
    LOWER QUARTILE     2.90000        3.42000
     MINIMUM VALUE     0.20000        0.11000
     MAXIMUM VALUE     22.20000        23.37000
```

```
SKILL OF PREDICTION PARAMETERS
CORRELATION COEFFICIENT OF PREDICTED
VERSUS OBSERVED   0.914
THE BOUNDS OF THE CORRELATION AT THE
CONFIDENCE LEVEL OF 0.050 ARE
LOW BOUND 0.891 HIGH BOUND 0.932
RATIO OF OVER TO UNDER PREDICTIONS  2.442
PERCENT OF OVER PREDICTIONS
GREATER THAN 200 PERCENT OF THE
OBSERVED   6.792
PERCENT OF UNDER PREDICTIONS
LESS THAN 50 PERCENT OF THE
OBSERVED   4.906
```

FIGURE A-1. RAPS UAM hourly ozone concentrations.

```
VARIABLE...OZONE
BEGINNING DATE...8/8/80
ENDING DATE...8/8/80
OBSERVATION SOURCE...OZONE
OBSERVATION ANALYSIS...AIRS DATA
THE PREDICTION ALGORITHM...UAM(CB-IV) OZONE
AVERAGING TIME...ALL HOURS
STRATITFYING VARIABLE...AIRS DATA SITES
SAMPLE SIZE...265
```



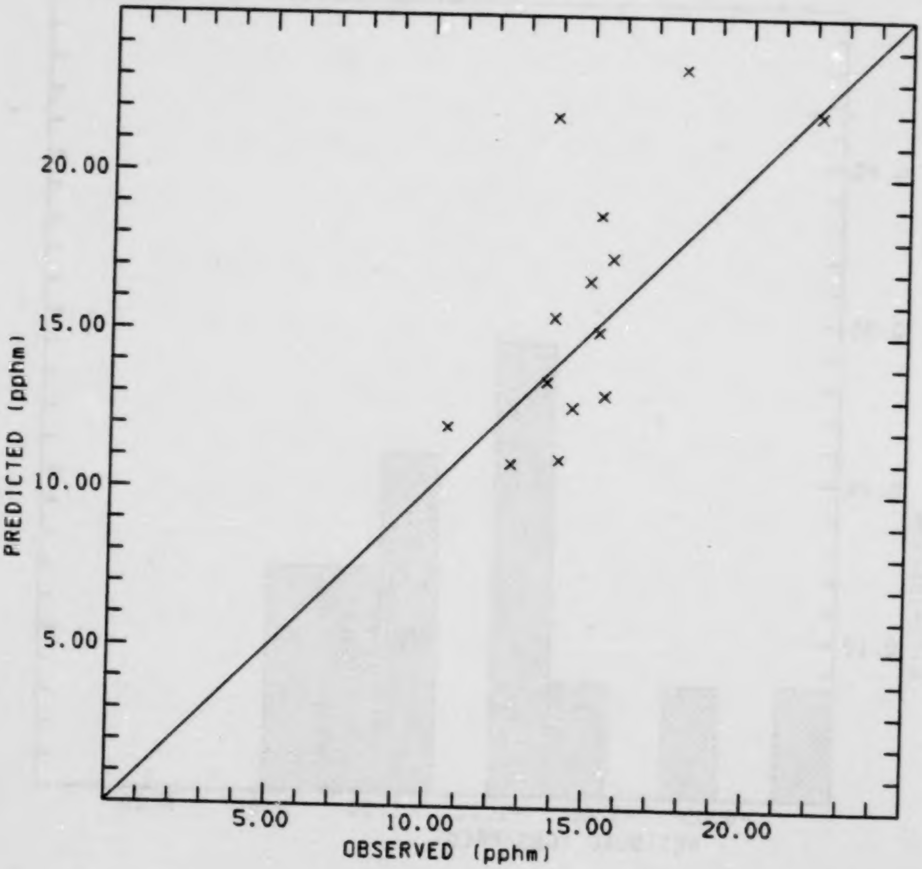
```
THE BINSIZE EQUALS  1.300

RESIDUAL ANALYSIS                         BIAS CONFIDENCE INTERVAL
          AVERAGE         -0.73835        AT THE 0.0500 LEVEL
   STANDARD DEVIATION      2.05125        LOWER BOUND -1.4451
           SKEWNESS        0.40933        UPPER BOUND -0.0316
           KURTOSIS        2.00005
     OTHER MEASURES                       STD RESIDUAL CONFIDENCE INTERVAL
           MEDIAN         -0.88000        AT THE 0.0500 LEVEL
      UPPER QUARTILE       0.25000        LOWER BOUND 3.6681
      LOWER QUARTILE      -1.92000        UPPER BOUND 4.8841
       MINIMUM VALUE      -8.62000
       MAXIMUM VALUE       7.36000        THE MEASURES OF GROSS ERROR
                                          THE ROOT MEAN SQUARE ERROR IS 2.18
                                          THE AVERAGE ABSOLUTE ERROR IS 1.67

                                          VARIOUS MEASURES OF RELATIVE VARIABILITY
                                          OBSERVATION COEFFICIENT OF VARIATION
                                                                    0.7168
                                          RESIDUAL COEFFICIENT OF VARIATION
                                                                    0.3026
                                          RATIO OF RESIDUAL TO OBSERVED ST. DEV.
                                                                    0.4222
```

FIGURE A-1. Concluded.

```
VARIABLE...OZONE
BEGINNING DATE...8/8/80
ENDING DATE...8/8/80
OBSERVATION SOURCE...OZONE
OBSERVATION ANALYSIS...AIRS DATA
THE PREDICTION ALGORITHM...UAM(CB-IV) OZONE
AVERAGING TIME...ALL HOURS
STRATITFYING VARIABLE...AIRS DATA SITES
SAMPLE SIZE...14
```

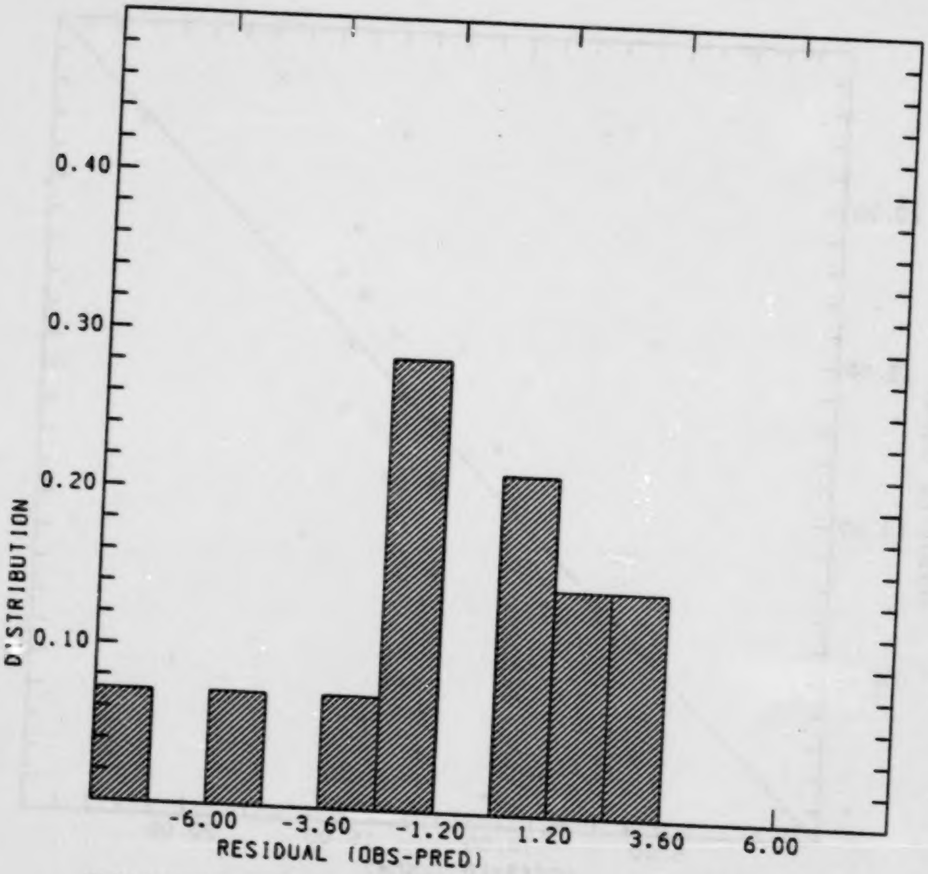


```
MOMENTS OF THE PROBABILITY DENSITY FUNCTION
                    OBSERVED      PREDICTED
       AVERAGE      15.01427       15.96999
 STANDARD DEVIATION 2.65243       4.18404
      SKEWNESS      1.10826       0.43840
      KURTOSIS      1.55511       -1.30929
   OTHER MEASURES
       MEDIAN       14.50000       15.06000
   UPPER QUARTILE   15.30000       17.39000
   LOWER QUARTILE   13.70000       12.02000
    MINIMUM VALUE   10.60000       10.87000
    MAXIMUM VALUE   22.20000       23.37000
```

```
SKILL OF PREDICTION PARAMETERS
CORRELATION COEFFICIENT OF PREDICTED
VERSUS OBSERVED   0.676
THE BOUNDS OF THE CORRELATION AT THE
CONFIDENCE LEVEL OF 0.050 ARE
LOW BOUND 0.227 HIGH BOUND 0.888
RATIO OF OVER TO UNDER PREDICTIONS  1.000
PERCENT OF OVER PREDICTIONS
GREATER THAN 200 PERCENT OF THE
OBSERVED   0.000
PERCENT OF UNDER PREDICTIONS
LESS THAN 50 PERCENT OF THE
OBSERVED   0.000
```

FIGURE A-2. RAPS UAM daily maximum ozone concentrations.

```
VARIABLE...OZONE
BEGINNING DATE...8/8/80
ENDING DATE...8/8/80
OBSERVATION SOURCE...OZONE
OBSERVATION ANALYSIS...AIRS DATA
THE PREDICTION ALGORITHM...UAM(CB-IV) OZONE
AVERAGING TIME...ALL HOURS
STRATITFYING VARIABLE...AIRS DATA SITES
SAMPLE SIZE...14
```



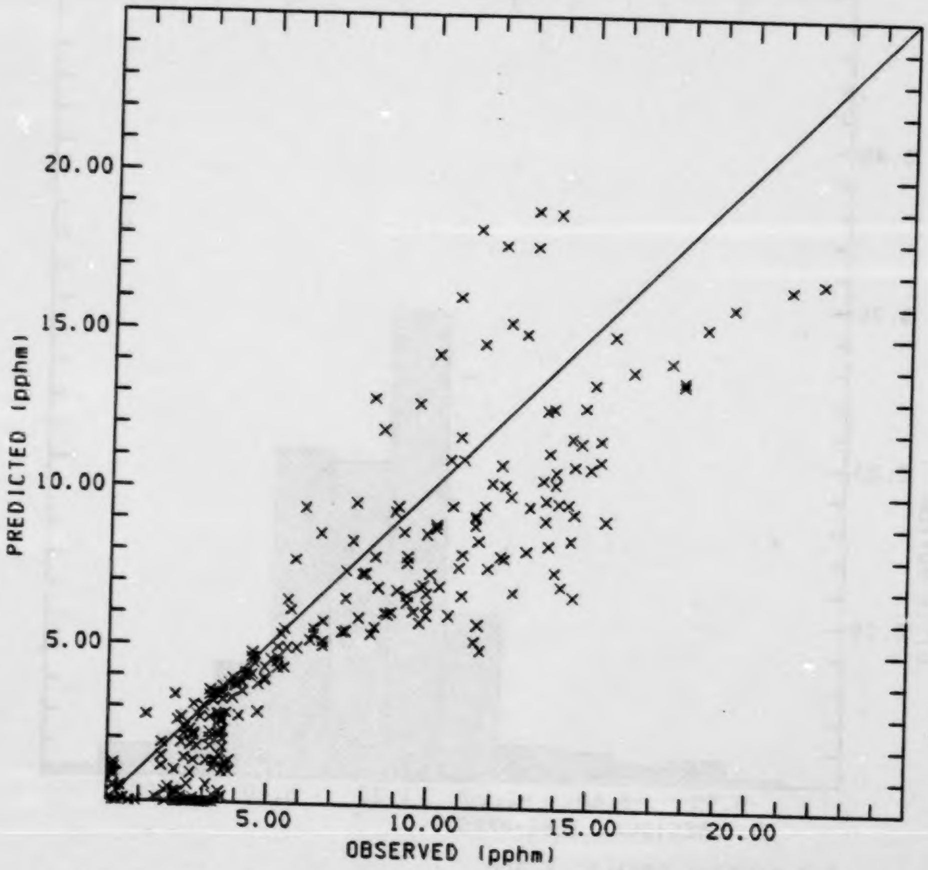
```
THE BINSIZE EQUALS  1.200

RESIDUAL ANALYSIS
                                           BIAS CONFIDENCE INTERVAL
          AVERAGE          -0.95571        AT THE 0.0500 LEVEL
   STANDARD DEVIATION       3.08663        LOWER BOUND -3.2883
          SKEWNESS         -0.71570        UPPER BOUND 1.3769
          KURTOSIS         -0.38413
    OTHER MEASURES                         STD RESIDUAL CONFIDENCE INTERVAL
          MEDIAN           -1.42000        AT THE 0.0500 LEVEL
     UPPER QUARTILE         0.26000        LOWER BOUND 5.6337
     LOWER QUARTILE        -3.43000        UPPER BOUND 20.3216
      MINIMUM VALUE        -7.92000
      MAXIMUM VALUE         3.08000        THE MEASURES OF GROSS ERROR
                                           THE ROOT MEAN SQUARE ERROR IS 3.12
                                           THE AVERAGE ABSOLUTE ERROR IS 2.36

                                           VARIOUS MEASURES OF RELATIVE VARIABILITY
                                           OBSERVATION COEFFICIENT OF VARIATION
                                                                          0.1767
                                           RESIDUAL COEFFICIENT OF VARIATION
                                                                          0.2056
                                           RATIO OF RESIDUAL TO OBSERVED ST. DEV.
                                                                          1.1637
```

FIGURE A-2. Concluded.

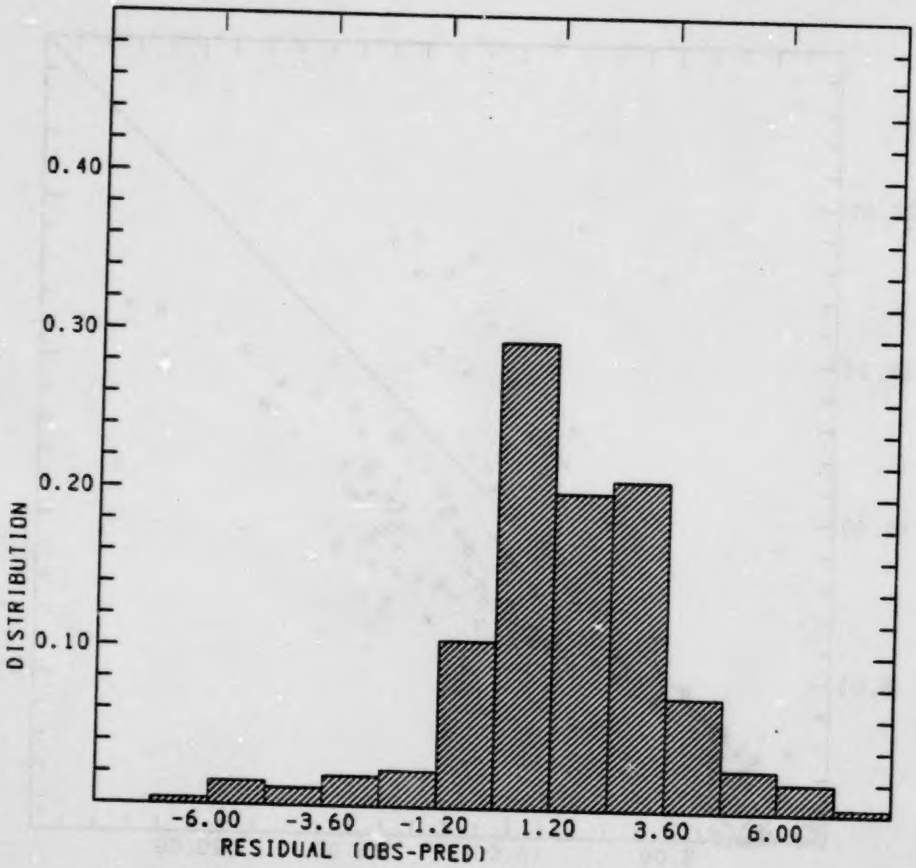
```
VARIABLE...OZONE
BEGINNING DATE...8/8/80
ENDING DATE...8/8/80
OBSERVATION SOURCE...OZONE
OBSERVATION ANALYSIS...AIRS DATA
THE PREDICTION ALGORITHM...PLANR UAM(CB-IV) OZONE
AVERAGING TIME...ALL HOURS
STRATITFYING VARIABLE...RAPS DATA SITES
SAMPLE SIZE...265
```



```
MOMENTS OF THE PROBABILITY DENSITY FUNCTION          SKILL OF PREDICTION PARAMETERS
                       OBSERVED        PREDICTED     CORRELATION COEFFICIENT OF PREDICTED
      AVERAGE           6.77843         5.35212      VERSUS OBSERVED    0.895
 STANDARD DEVIATION     4.85895         4.62851      THE BOUNDS OF THE CORRELATION AT THE
      SKEWNESS          0.68694         0.80435      CONFIDENCE LEVEL OF 0.050 ARE
      KURTOSIS         -0.47257         -0.04013     LOW BOUND 0.868 HIGH BOUND 0.916
   OTHER MEASURES                                    RATIO OF OVER TO UNDER PREDICTIONS  0.221
      MEDIAN            4.90000         4.30000      PERCENT OF OVER PREDICTIONS
   UPPER QUARTILE      10.60000          8.30000     GREATER THAN 200 PERCENT OF THE
   LOWER QUARTILE       2.90000         1.32000      OBSERVED    2.642
    MINIMUM VALUE       0.20000         0.01000      PERCENT OF UNDER PREDICTIONS
    MAXIMUM VALUE      22.20000         18.87000     LESS THAN 50 PERCENT OF THE
                                                     OBSERVED    24.906
```

FIGURE A-3. PLANR UAM hourly ozone concentrations.

```
VARIABLE...OZONE
BEGINNING DATE...8/8/80
ENDING DATE...8/8/80
OBSERVATION SOURCE...OZONE
OBSERVATION ANALYSIS...AIRS DATA
THE PREDICTION ALGORITHM...PLANR UAM(CB-IV) OZONE
AVERAGING TIME...ALL HOURS
STRATITFYING VARIABLE...RAPS DATA SITES
SAMPLE SIZE...265
```



```
THE BINSIZE EQUALS  1.200
```

```
RESIDUAL ANALYSIS

         AVERAGE            1.42629
  STANDARD DEVIATION        2.18869
          SKEWNESS         -0.47534
          KURTOSIS          1.75804
    OTHER MEASURES
           MEDIAN           1.37000
      UPPER QUARTILE        2.69000
      LOWER QUARTILE        0.20000
       MINIMUM VALUE       -6.86000
       MAXIMUM VALUE        7.80000
```

```
BIAS CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND 0.7457
UPPER BOUND 2.1069

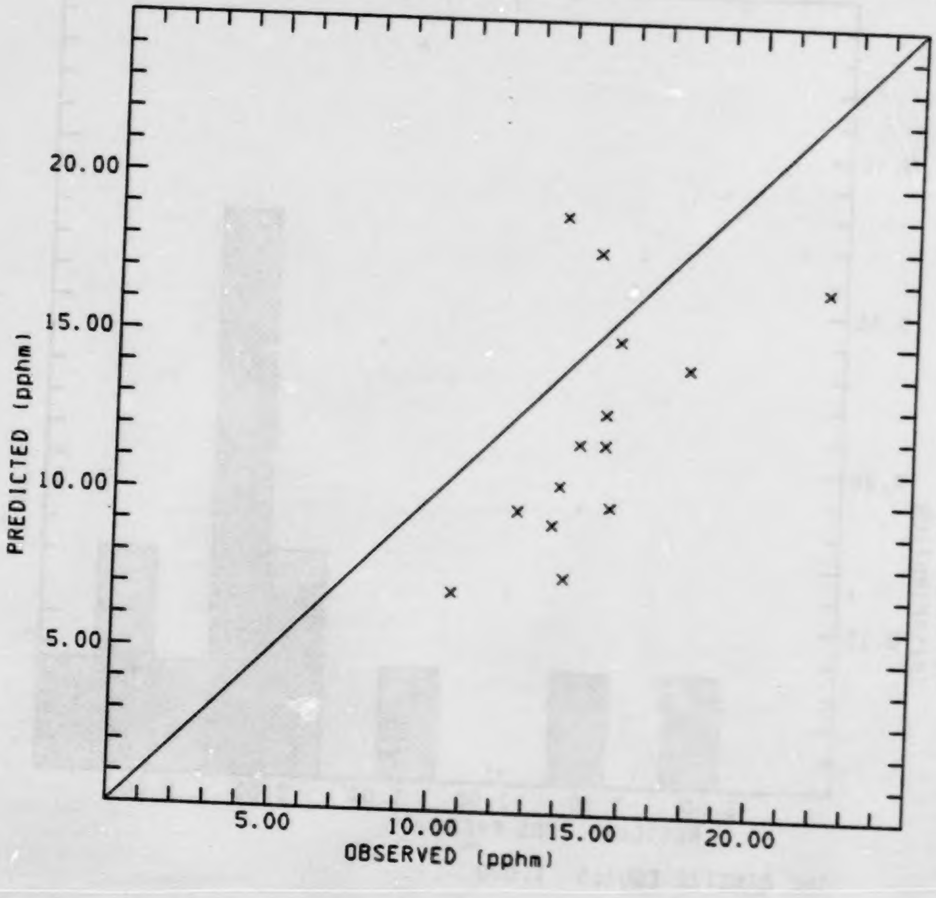
STD RESIDUAL CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND 4.1761
UPPER BOUND 5.5605

THE MEASURES OF GROSS ERROR
THE ROOT MEAN SQUARE ERROR IS 2.61
THE AVERAGE ABSOLUTE ERROR IS 2.02

VARIOUS MEASURES OF RELATIVE VARIABILITY
OBSERVATION COEFFICIENT OF VARIATION
                               0.7168
RESIDUAL COEFFICIENT OF VARIATION
                               0.3229
RATIO OF RESIDUAL TO OBSERVED ST. DEV.
                               0.4504
```

FIGURE A-3. Concluded.

```
VARIABLE...OZONE
BEGINNING DATE...8/8/80
ENDING DATE...8/8/80
OBSERVATION SOURCE...OZONE
OBSERVATION ANALYSIS...AIRS DATA
THE PREDICTION ALGORITHM...PLANR UAM(CB-IV) OZONE
AVERAGING TIME...ALL HOURS
STRATITFYING VARIABLE...RAPS DATA SITES
SAMPLE SIZE...14
```

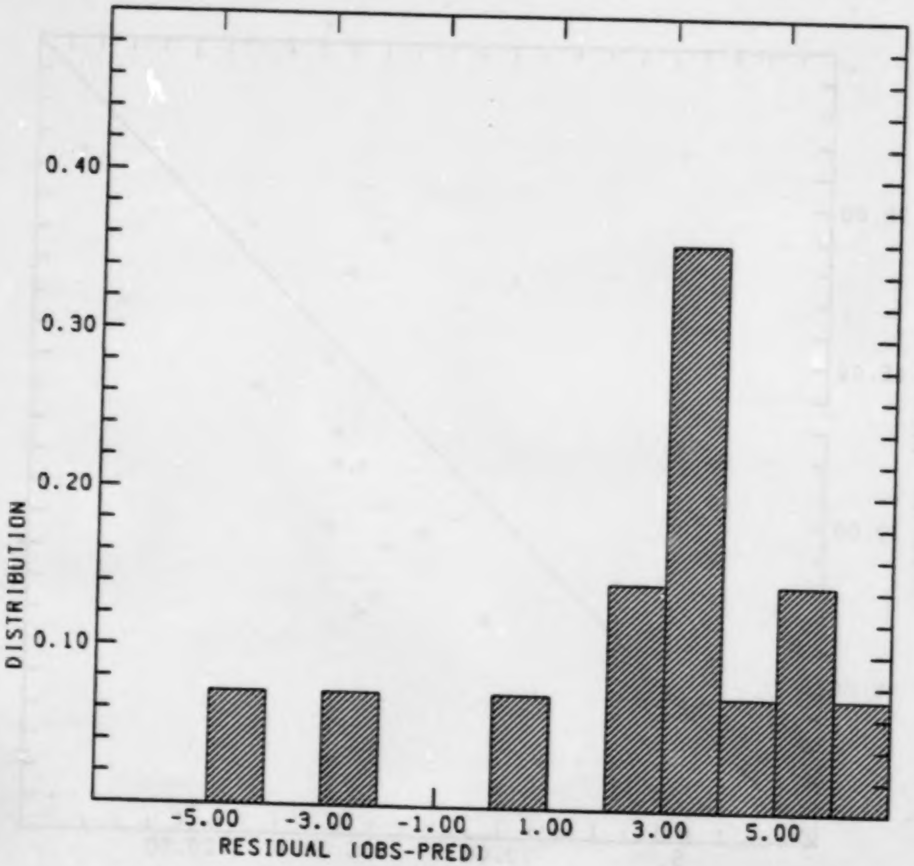


```
MOMENTS OF THE PROBABILITY DENSITY FUNCTION
                        OBSERVED       PREDICTED
         AVERAGE        15.01427       12.26499
  STANDARD DEVIATION     2.65243        3.75908
         SKEWNESS        1.10826        0.30977
         KURTOSIS        1.55511       -1.27994
   OTHER MEASURES
          MEDIAN        14.50000       11.69000
   UPPER QUARTILE       15.30000       14.15000
   LOWER QUARTILE       13.70000        9.14000
   MINIMUM VALUE        10.60000        6.93000
   MAXIMUM VALUE        22.20000       18.87000
```

```
SKILL OF PREDICTION PARAMETERS
CORRELATION COEFFICIENT OF PREDICTED
VERSUS OBSERVED   0.550
THE BOUNDS OF THE CORRELATION AT THE
CONFIDENCE LEVEL OF 0.050 ARE
LOW BOUND 0.027 HIGH BOUND 0.837
RATIO OF OVER TO UNDER PREDICTIONS  0.167
PERCENT OF OVER PREDICTIONS
GREATER THAN 200 PERCENT OF THE
OBSERVED   0.000
PERCENT OF UNDER PREDICTIONS
LESS THAN 50 PERCENT OF THE
OBSERVED   0.000
```

FIGURE A-4. PLANR UAM daily maximum ozone concentrations.

```
VARIABLE...OZONE
BEGINNING DATE...8/8/80
ENDING DATE...8/8/80
OBSERVATION SOURCE...OZONE
OBSERVATION ANALYSIS...AIRS DATA
THE PREDICTION ALGORITHM...PLANR UAM(CB-IV) OZONE
AVERAGING TIME...ALL HOURS
STRATITFYING VARIABLE...RAPS DATA SITES
SAMPLE SIZE...14
```



```
THE BINSIZE EQUALS  1.000

RESIDUAL ANALYSIS
          AVERAGE            2.74929
   STANDARD DEVIATION        3.19348
          SKEWNESS          -1.13820
          KURTOSIS           0.34709
     OTHER MEASURES
          MEDIAN             3.53000
     UPPER QUARTILE          3.75000
     LOWER QUARTILE          0.72000
      MINIMUM VALUE         -4.97000
      MAXIMUM VALUE          6.64000

BIAS CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND 0.5831
UPPER BOUND 4.9155

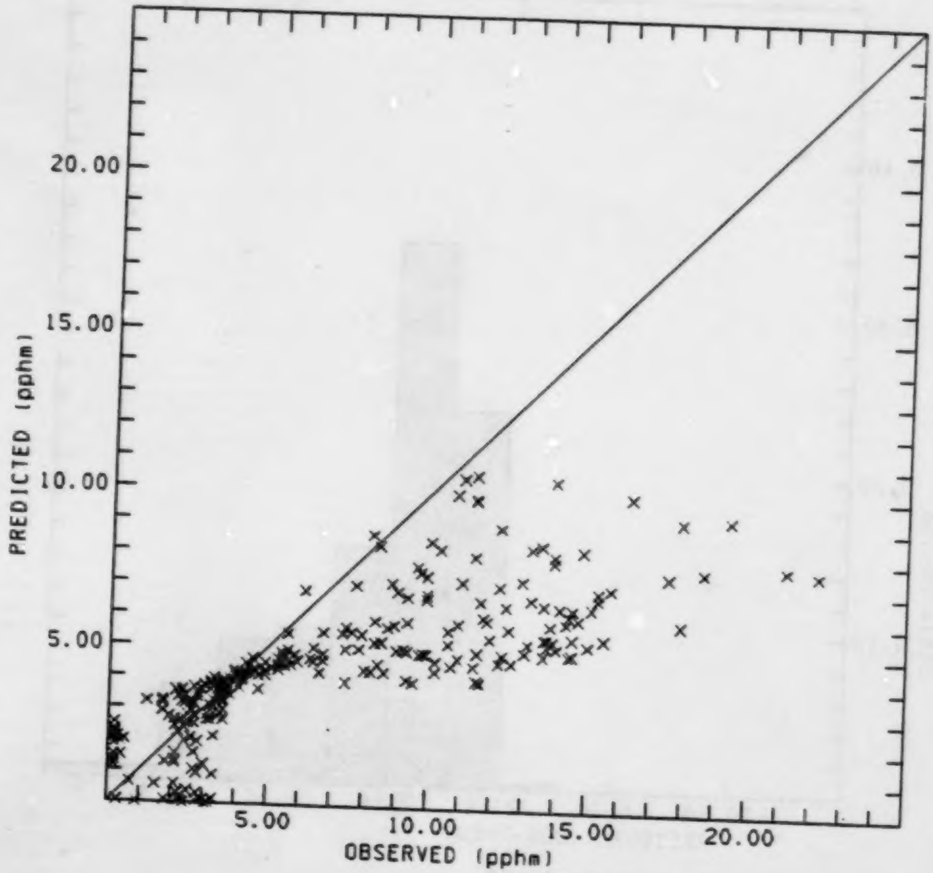
STD RESIDUAL CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND 6.0305
UPPER BOUND 21.7528

THE MEASURES OF GROSS ERROR
THE ROOT MEAN SQUARE ERROR IS 4.13
THE AVERAGE ABSOLUTE ERROR IS 3.85

VARIOUS MEASURES OF RELATIVE VARIABILITY
OBSERVATION COEFFICIENT OF VARIATION
                                0.1767
RESIDUAL COEFFICIENT OF VARIATION
                                0.2127
RATIO OF RESIDUAL TO OBSERVED ST. DEV.
                                1.2040
```

FIGURE A-4. Concluded.

```
VARIABLE...OZONE
BEGINNING DATE...8/8/80
ENDING DATE...8/8/80
OBSERVATION SOURCE...OZONE
OBSERVATION ANALYSIS...AIRS DATA
THE PREDICTION ALGORITHM...SIMPLE UAM(CB-IV) OZONE
AVERAGING TIME...ALL HOURS
STRATITFYING VARIABLE...RAPS DATA SITES
SAMPLE SIZE...265
```

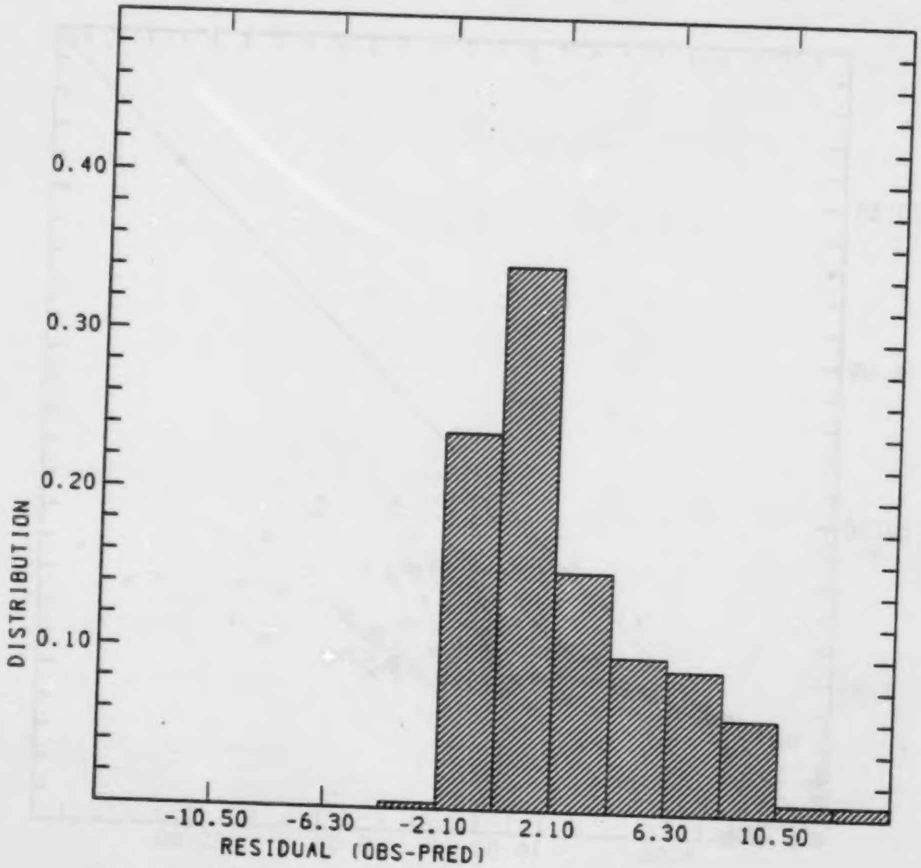


```
MOMENTS OF THE PROBABILITY DENSITY FUNCTION
                      OBSERVED       PREDICTED
        AVERAGE       6.77843        4.32029
 STANDARD DEVIATION   4.85895        2.23995
        SKEWNESS      0.68694        0.33689
        KURTOSIS     -0.47257         0.12427
   OTHER MEASURES
        MEDIAN        4.90000        4.20000
    UPPER QUARTILE    10.60000        5.45000
    LOWER QUARTILE    2.90000        2.95000
     MINIMUM VALUE    0.20000        0.01000
     MAXIMUM VALUE    22.20000        10.56000
```

```
SKILL OF PREDICTION PARAMETERS
CORRELATION COEFFICIENT OF PREDICTED
VERSUS OBSERVED   0.793
THE BOUNDS OF THE CORRELATION AT THE
CONFIDENCE LEVEL OF 0.050 ARE
LOW BOUND 0.743 HIGH BOUND 0.833
RATIO OF OVER TO UNDER PREDICTIONS  0.318
PERCENT OF OVER PREDICTIONS
GREATER THAN 200 PERCENT OF THE
OBSERVED   6.038
PERCENT OF UNDER PREDICTIONS
LESS THAN 50 PERCENT OF THE
OBSERVED   27.170
```

FIGURE A-5. SIMPLE UAM hourly ozone concentrations.

```
VARIABLE...OZONE
BEGINNING DATE...8/8/80
ENDING DATE...8/8/80
OBSERVATION SOURCE...OZONE
OBSERVATION ANALYSIS...AIRS DATA
THE PREDICTION ALGORITHM...SIMPLE UAM(CB-IV) OZONE
AVERAGING TIME...ALL HOURS
STRATITFYING VARIABLE...RAPS DATA SITES
SAMPLE SIZE...265
```



```
THE BINSIZE EQUALS 2.100

RESIDUAL ANALYSIS
             AVERAGE       2.45812
    STANDARD DEVIATION     3.37279
            SKEWNESS       1.01240
            KURTOSIS       0.26181
     OTHER MEASURES
             MEDIAN        1.10000
       UPPER QUARTILE      4.35000
       LOWER QUARTILE      0.01000
        MINIMUM VALUE     -2.31000
        MAXIMUM VALUE     14.57000

BIAS CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND 1.9155
UPPER BOUND 3.0008

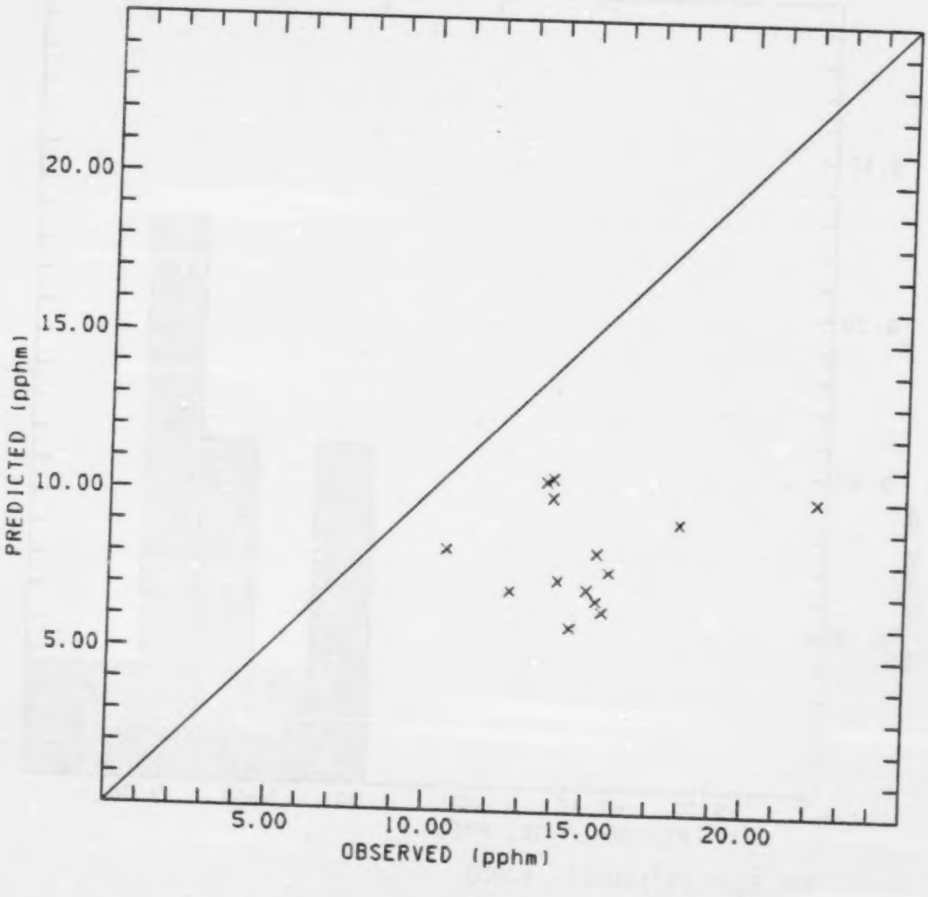
STD RESIDUAL CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND 9.9170
UPPER BOUND 13.2046

THE MEASURES OF GROSS ERROR
THE ROOT MEAN SQUARE ERROR IS 4.17
THE AVERAGE ABSOLUTE ERROR IS 2.85

VARIOUS MEASURES OF RELATIVE VARIABILITY
OBSERVATION COEFFICIENT OF VARIATION
                                  0.7168
RESIDUAL COEFFICIENT OF VARIATION
                                  0.4976
RATIO OF RESIDUAL TO OBSERVED ST. DEV.
                                  0.6941
```

FIGURE A-5. Concluded.

```
VARIABLE...OZONE
BEGINNING DATE...8/8/80
ENDING DATE...8/8/80
OBSERVATION SOURCE...OZONE
OBSERVATION ANALYSIS...AIRS DATA
THE PREDICTION ALGORITHM...SIMPLE UAM(CB-IV) OZONE
AVERAGING TIME...ALL HOURS
STRATITFYING VARIABLE...RAPS DATA SITES
SAMPLE SIZE...14
```

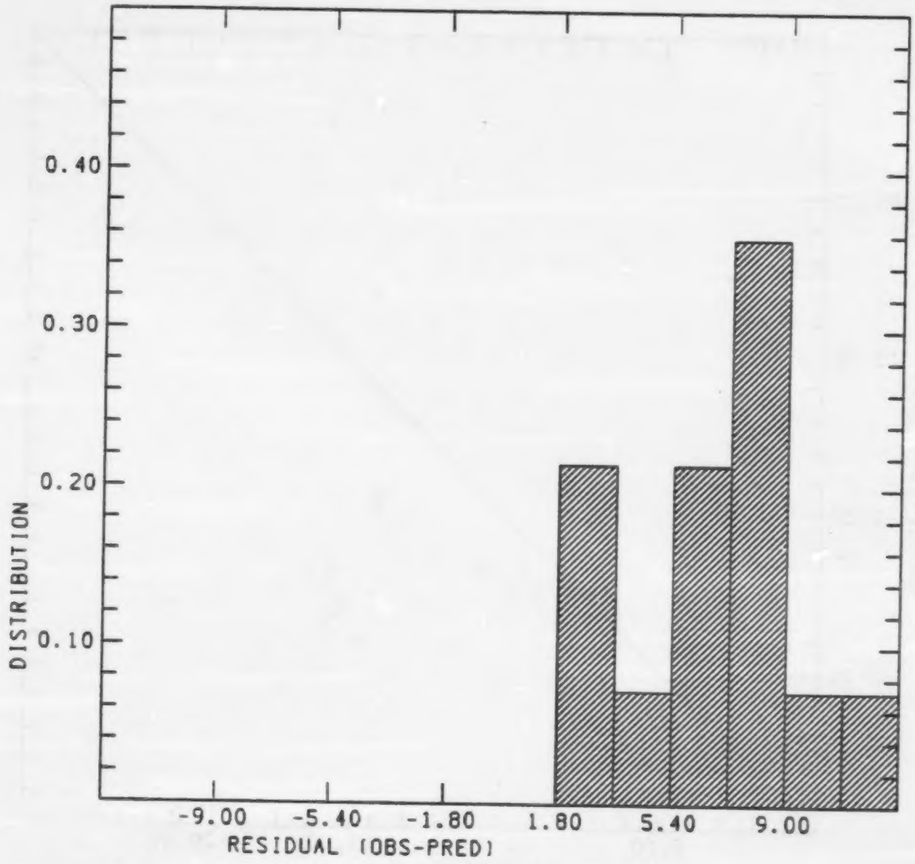


```
MOMENTS OF THE PROBABILITY DENSITY FUNCTION
                        OBSERVED       PREDICTED
          AVERAGE       15.01427        8.17999
 STANDARD DEVIATION      2.65243        1.58534
          SKEWNESS       1.10826        0.20928
          KURTOSIS       1.55511       -1.54830
   OTHER MEASURES
           MEDIAN       14.50000        7.63000
    UPPER QUARTILE      15.30000        9.19000
    LOWER QUARTILE      13.70000        6.71000
     MINIMUM VALUE      10.60000        5.85000
     MAXIMUM VALUE      22.20000       10.56000
```

```
SKILL OF PREDICTION PARAMETERS
CORRELATION COEFFICIENT OF PREDICTED
VERSUS OBSERVED    0.199
THE BOUNDS OF THE CORRELATION AT THE
CONFIDENCE LEVEL OF 0.050 ARE
LOW BOUND -0.371 HIGH BOUND 0.660
RATIO OF OVER TO UNDER PREDICTIONS  0.000
PERCENT OF OVER PREDICTIONS
GREATER THAN 200 PERCENT OF THE
OBSERVED    0.000
PERCENT OF UNDER PREDICTIONS
LESS THAN 50 PERCENT OF THE
OBSERVED    42.857
```

FIGURE A-6. SIMPLE UAM daily maximum ozone concentrations.

```
VARIABLE...OZONE
BEGINNING DATE...8/8/80
ENDING DATE...8/8/80
OBSERVATION SOURCE...OZONE
OBSERVATION ANALYSIS...AIRS DATA
THE PREDICTION ALGORITHM...SIMPLE UAM(CB-IV) OZONE
AVERAGING TIME...ALL HOURS
STRATITFYING VARIABLE...RAPS DATA SITES
SAMPLE SIZE...14
```



```
THE BINSIZE EQUALS  1.800
```

```
RESIDUAL ANALYSIS

           AVERAGE          6.83428
  STANDARD DEVIATION        2.80639
          SKEWNESS         -0.04242
          KURTOSIS         -1.02145
     OTHER MEASURES
            MEDIAN          7.08000
      UPPER QUARTILE        8.59000
      LOWER QUARTILE        3.34000
       MINIMUM VALUE        2.34000
       MAXIMUM VALUE       12.25000
```

```
BIAS CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND 5.3793
UPPER BOUND 8.2893

STD RESIDUAL CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND 4.6571
UPPER BOUND 16.7990

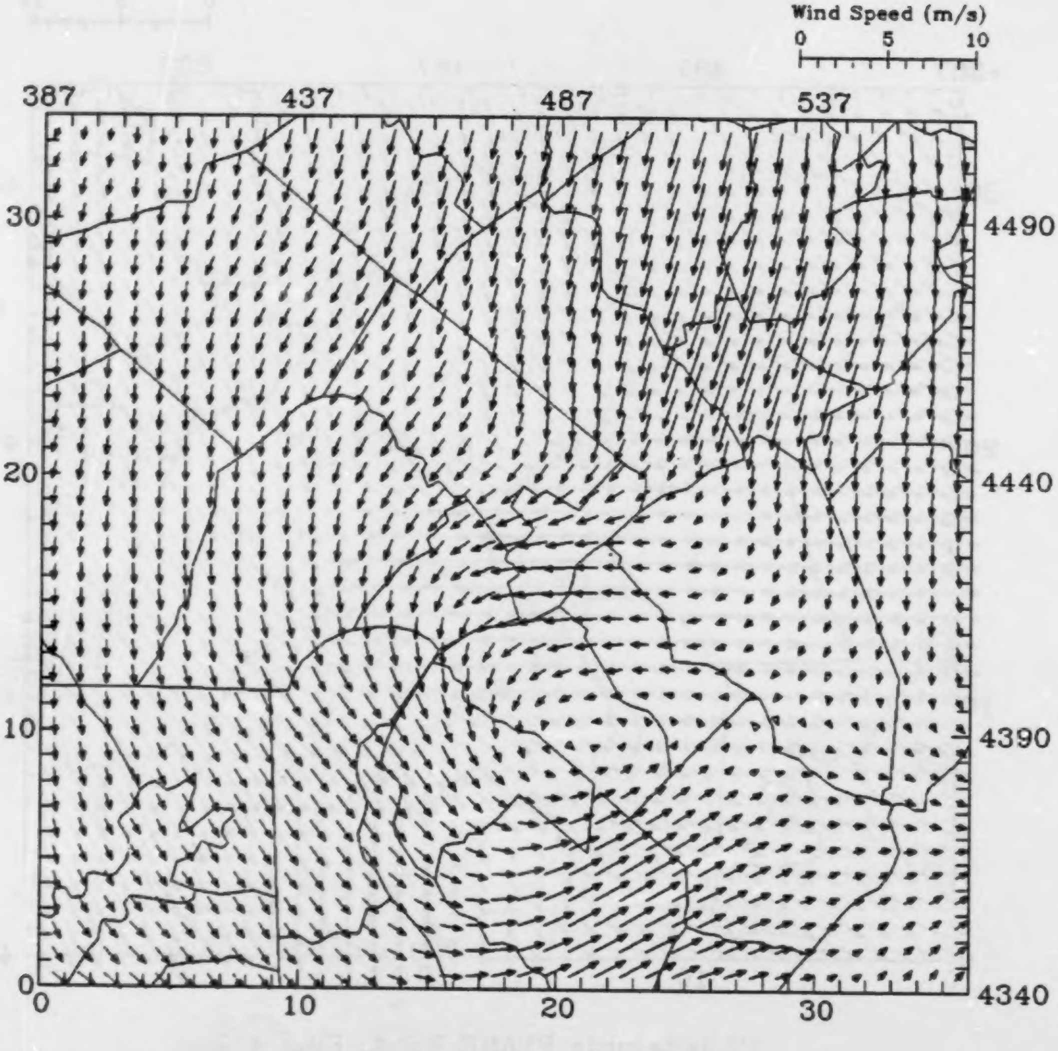
THE MEASURES OF GROSS ERROR
THE ROOT MEAN SQUARE ERROR IS 7.35
THE AVERAGE ABSOLUTE ERROR IS 6.83

VARIOUS MEASURES OF RELATIVE VARIABILITY
OBSERVATION COEFFICIENT OF VARIATION
                                0.1767
RESIDUAL COEFFICIENT OF VARIATION
                                0.1869
RATIO OF RESIDUAL TO OBSERVED ST. DEV.
                                1.0580
```

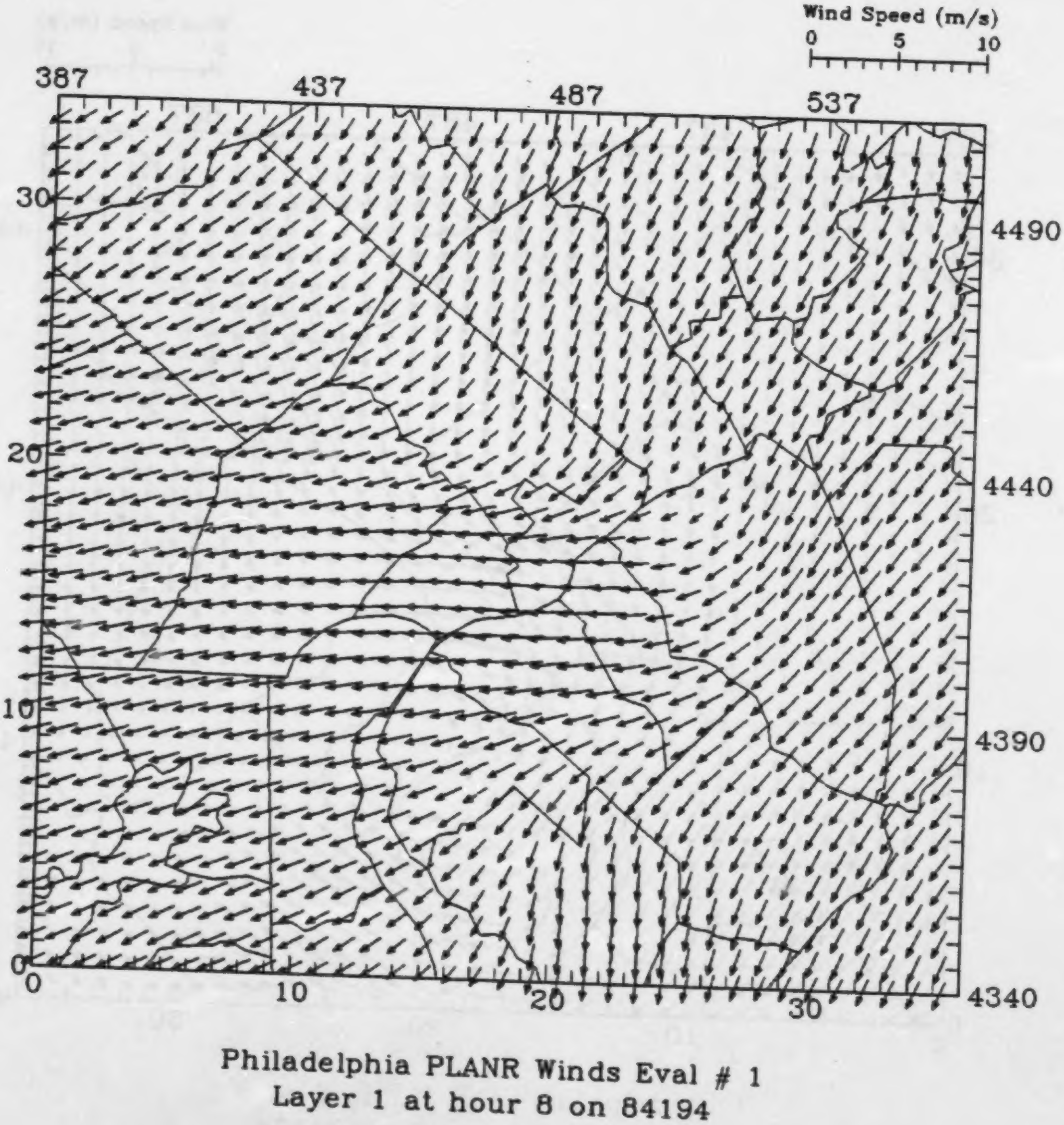
FIGURE A-6. Concluded.

Appendix B

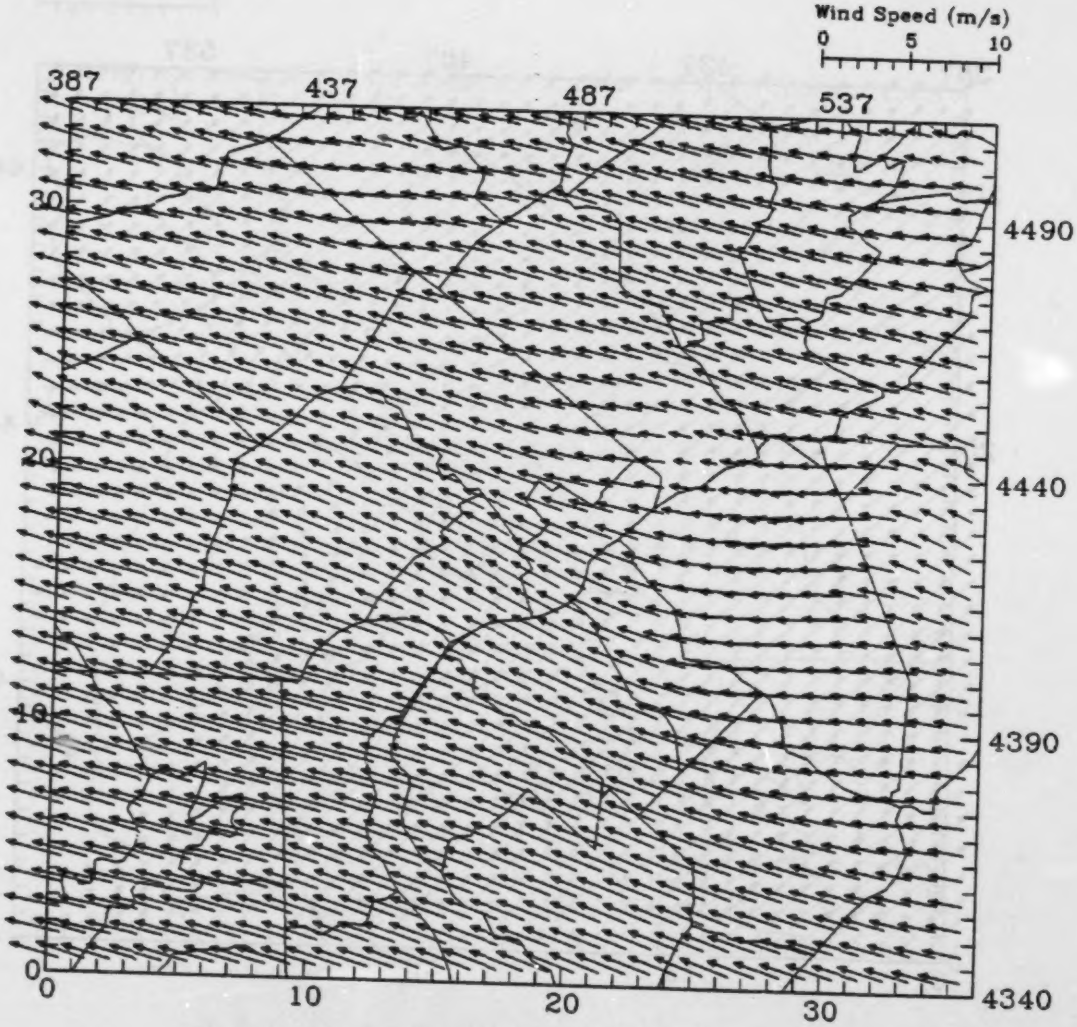
WIND FIELDS USED IN DIAGNOSTIC RUN 1 APPLICATION TO PHILADELPHIA


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

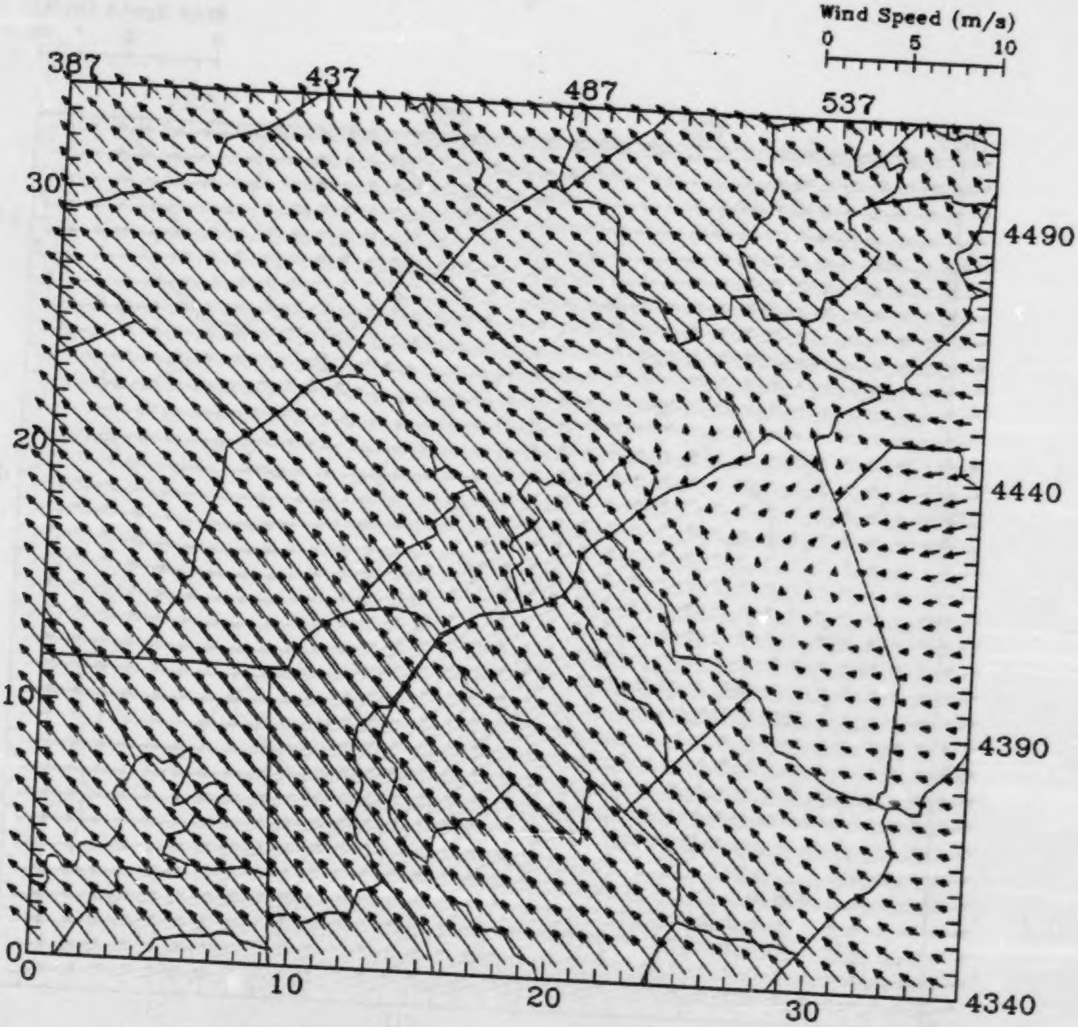
Philadelphia PLANR Winds Eval # 1
Layer 1 at hour 7 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

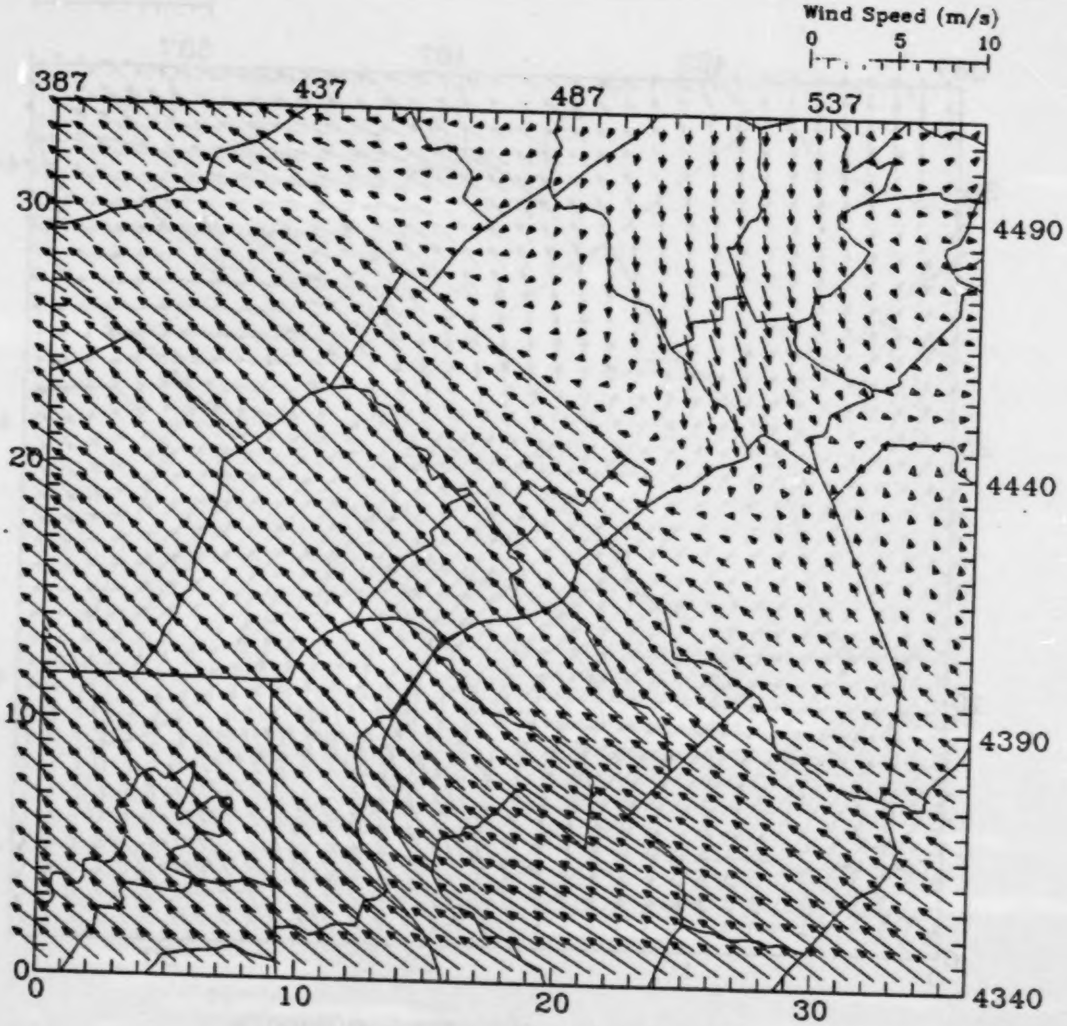
Philadelphia PLANR Winds Eval # 1
Layer 1 at hour 8 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

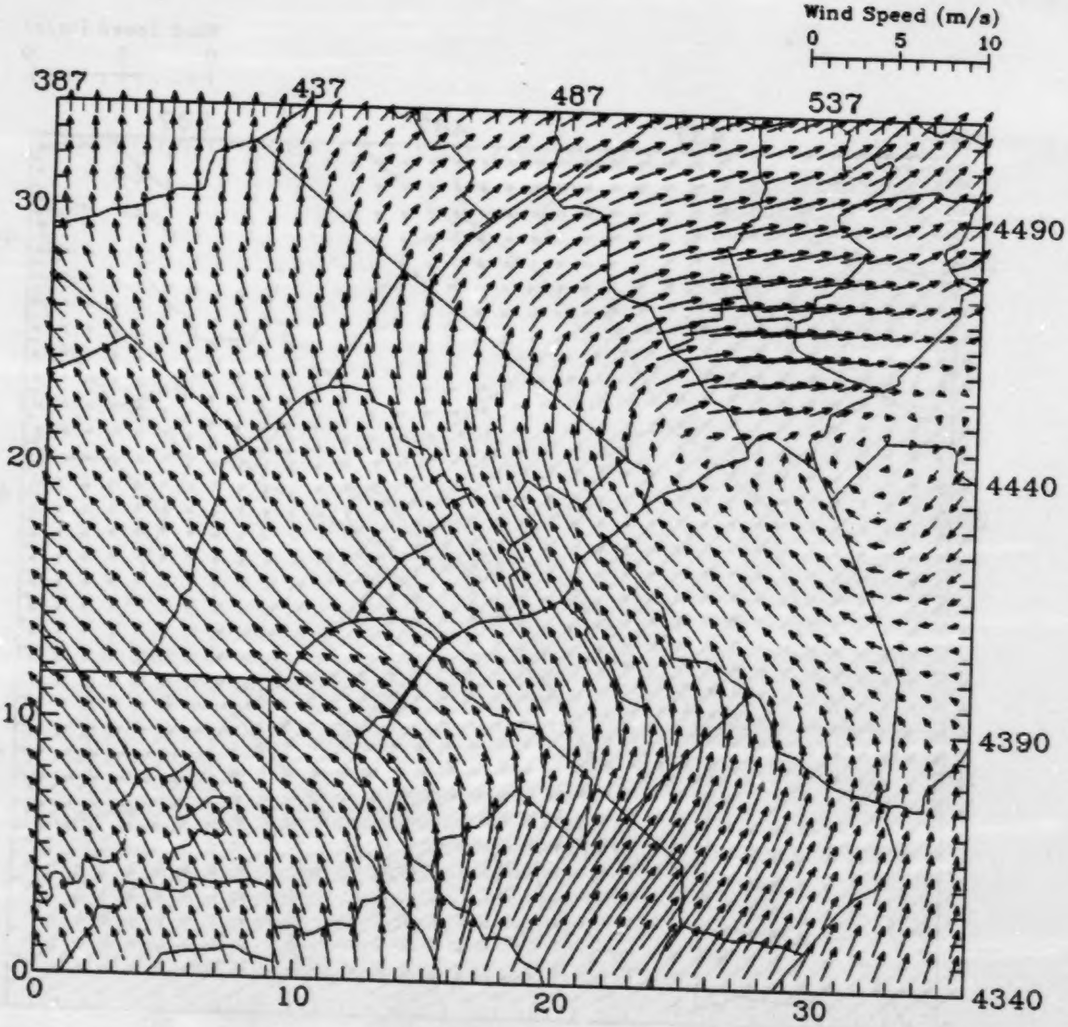
Philadelphia PLANR Winds Eval # 1
Layer 1 at hour 9 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

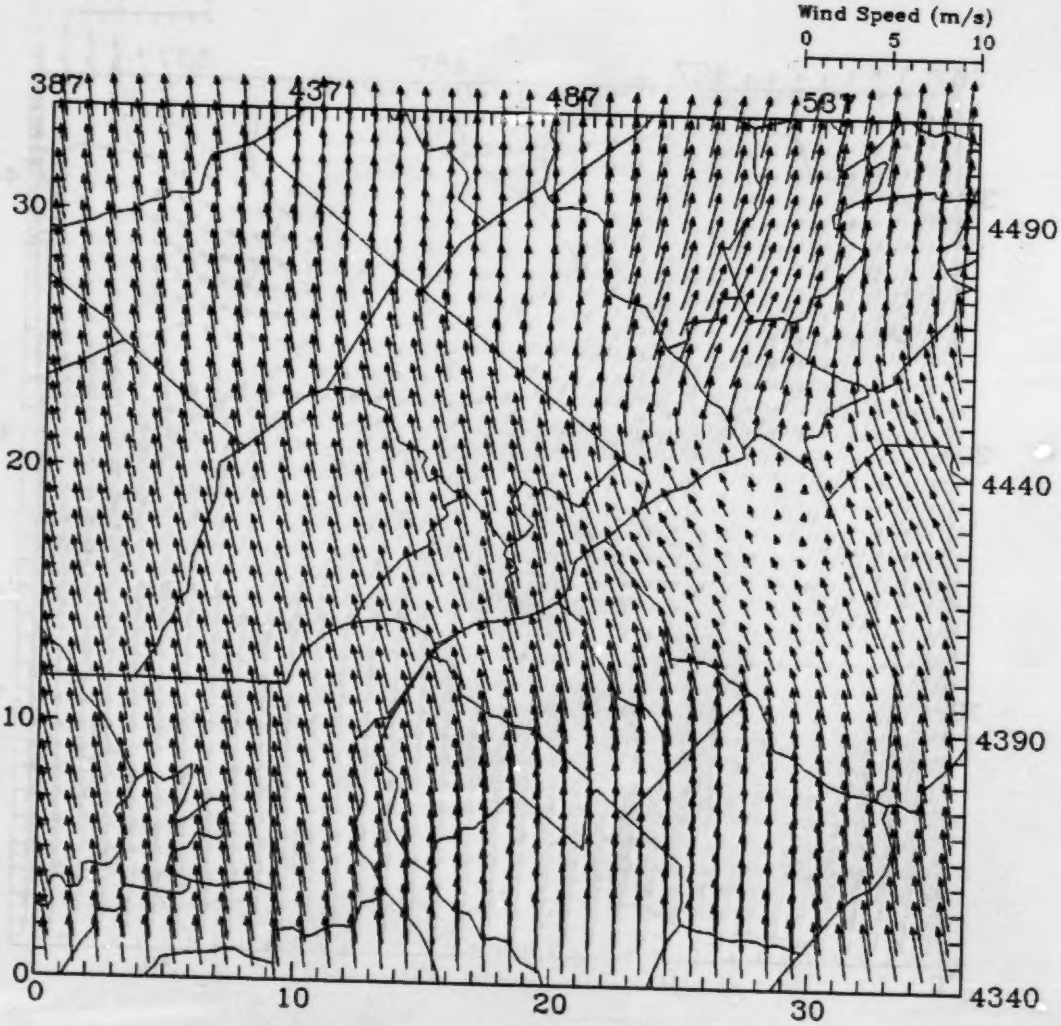
Philadelphia PLANR Winds Eval # 1
Layer 1 at hour 10 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
4490
4440
4390
4340
0
10
20
30

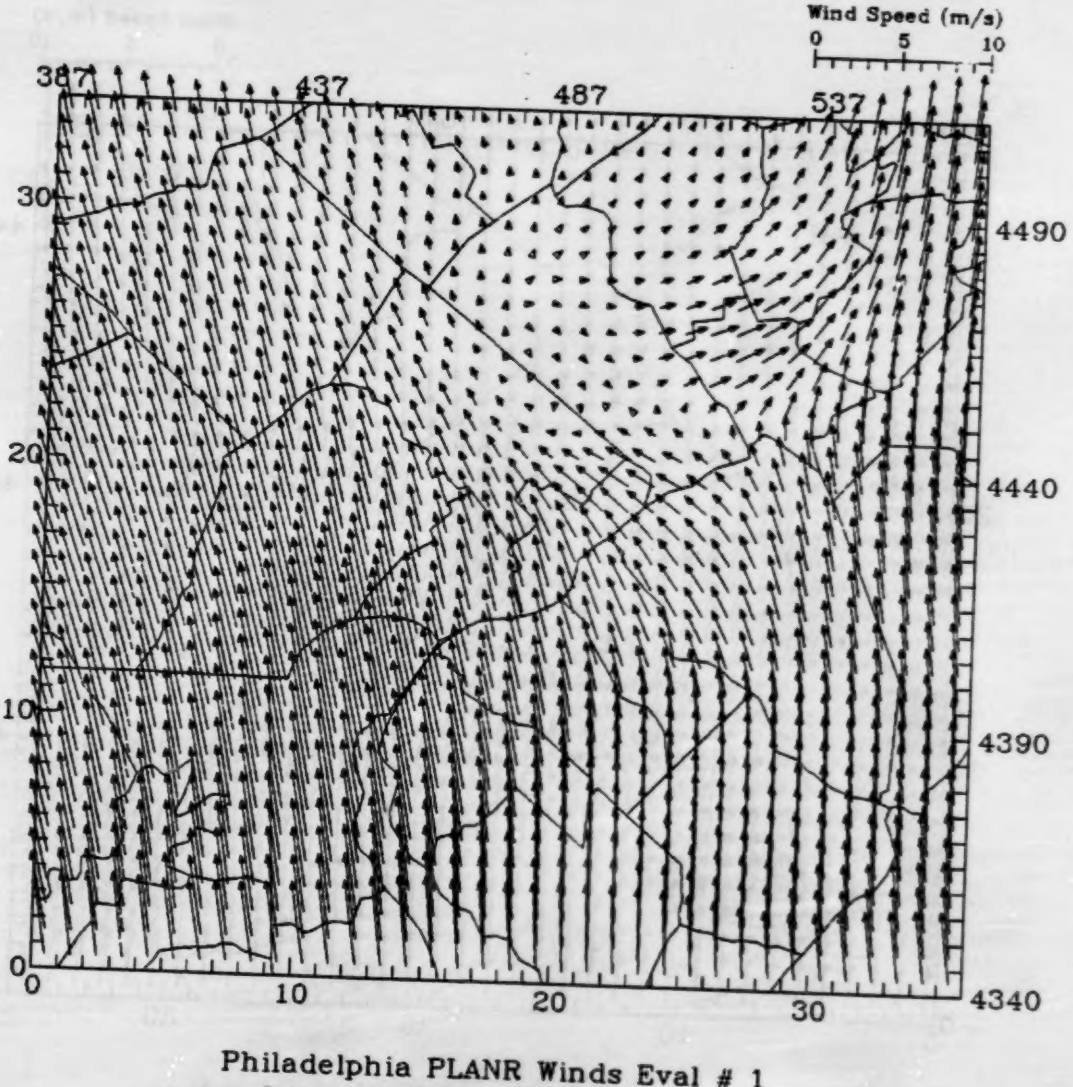
Philadelphia PLANR Winds Eval # 1
Layer 1 at hour 11 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
4490
4440
4390
4340
0
10
20
30

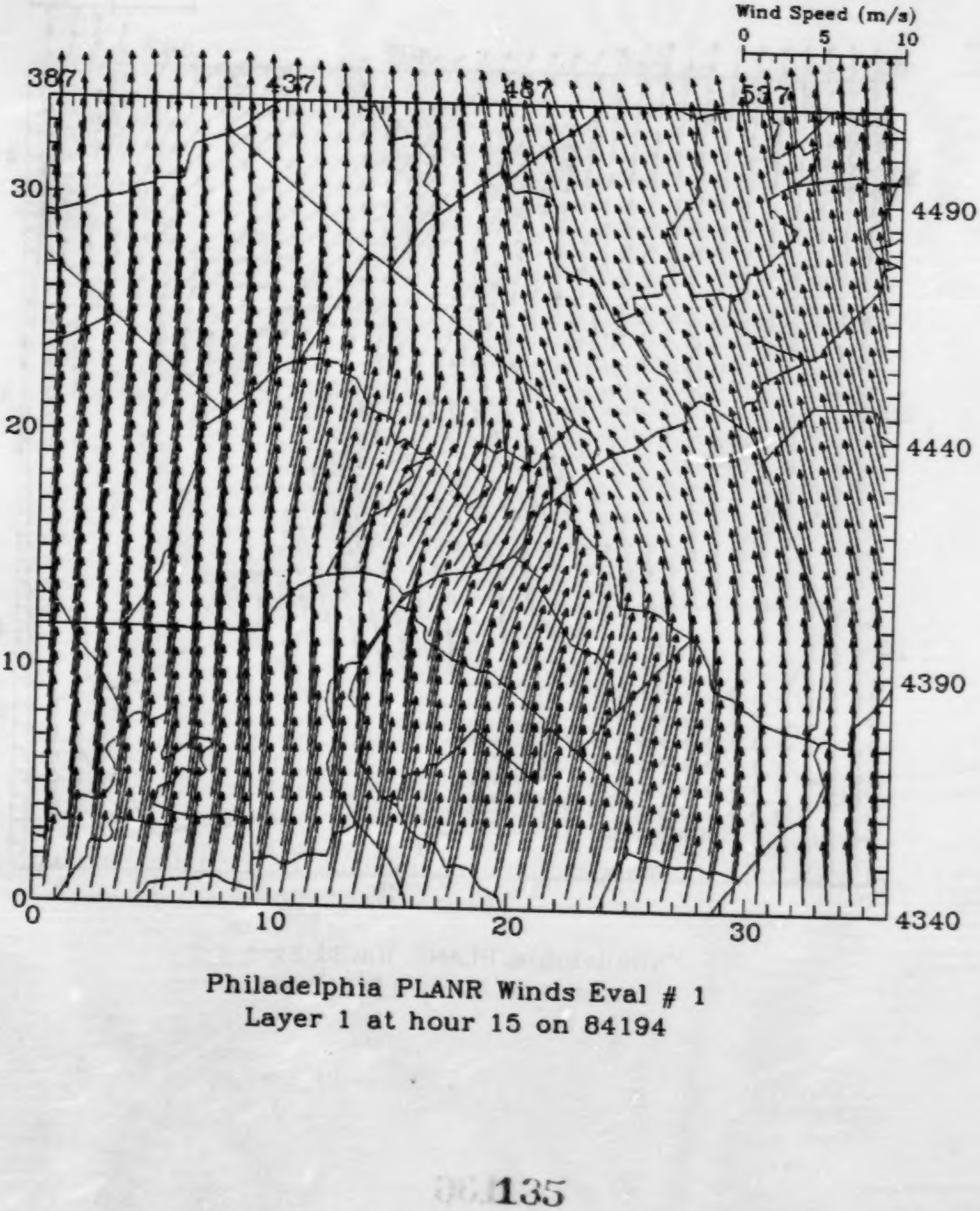
Philadelphia PLANR Winds Eval # 1
Layer 1 at hour 12 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

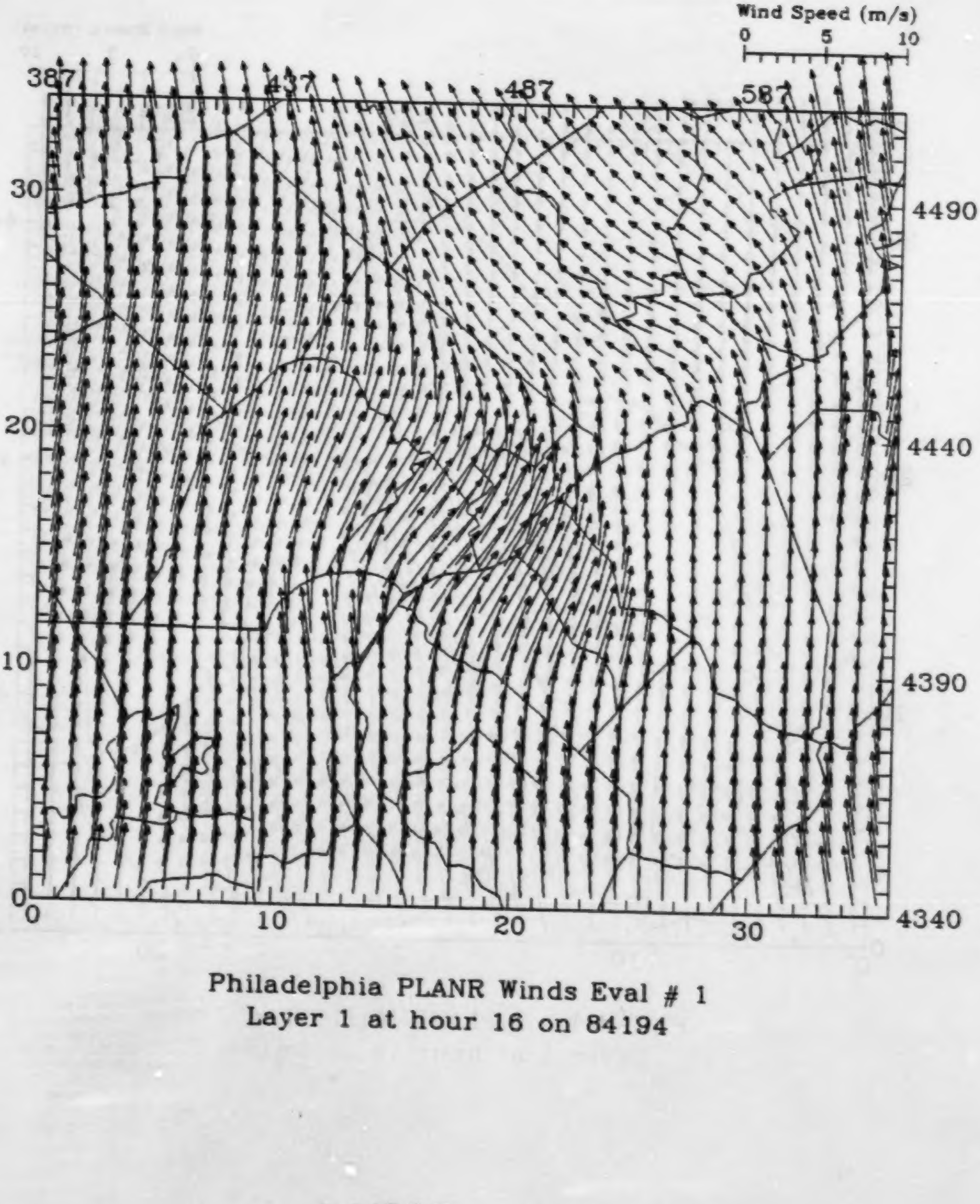
Philadelphia PLANR Winds Eval # 1
Layer 1 at hour 13 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

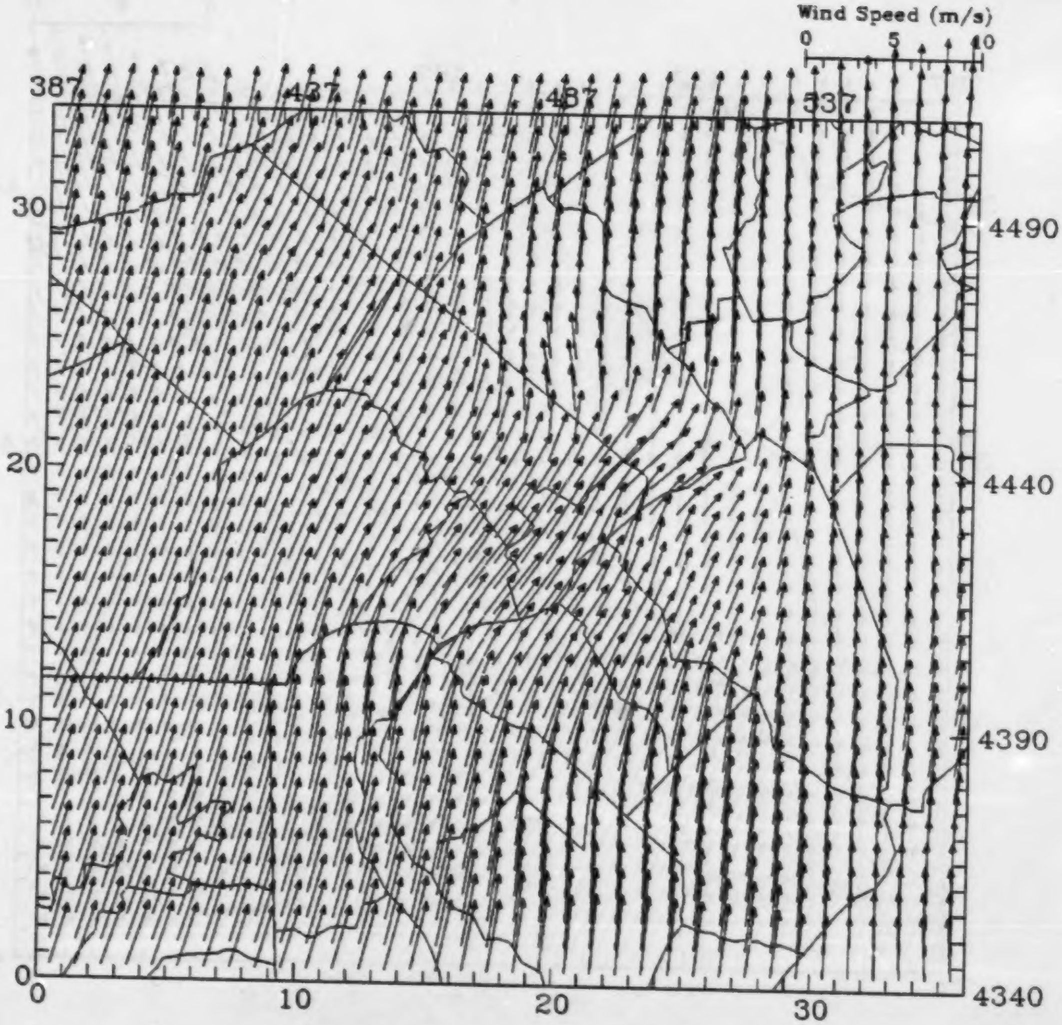
Philadelphia PLANR Winds Eval # 1
Layer 1 at hour 14 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

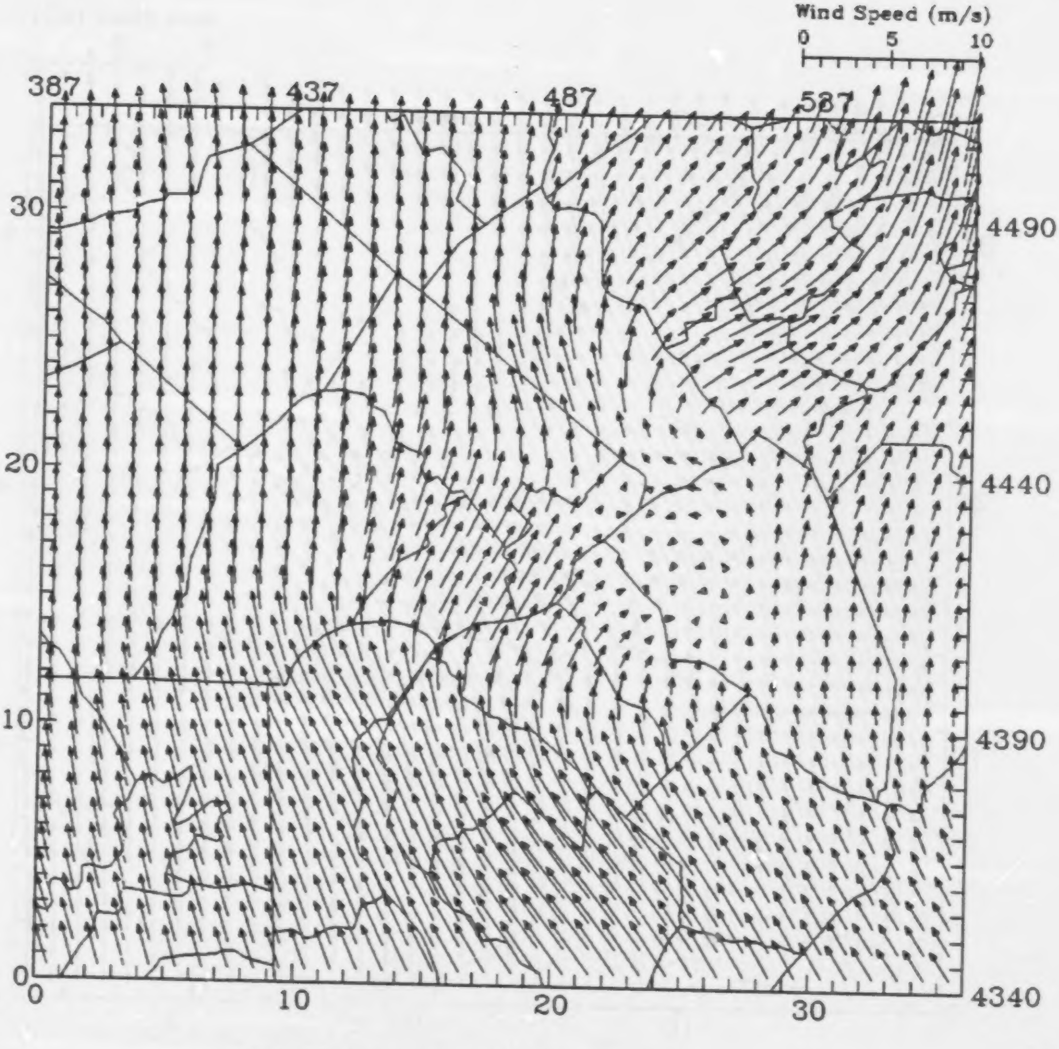
Philadelphia PLANR Winds Eval # 1
Layer 1 at hour 15 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
587
30
20
10
0
0
10
20
30
4490
4440
4390
4340

Philadelphia PLANR Winds Eval # 1
Layer 1 at hour 16 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

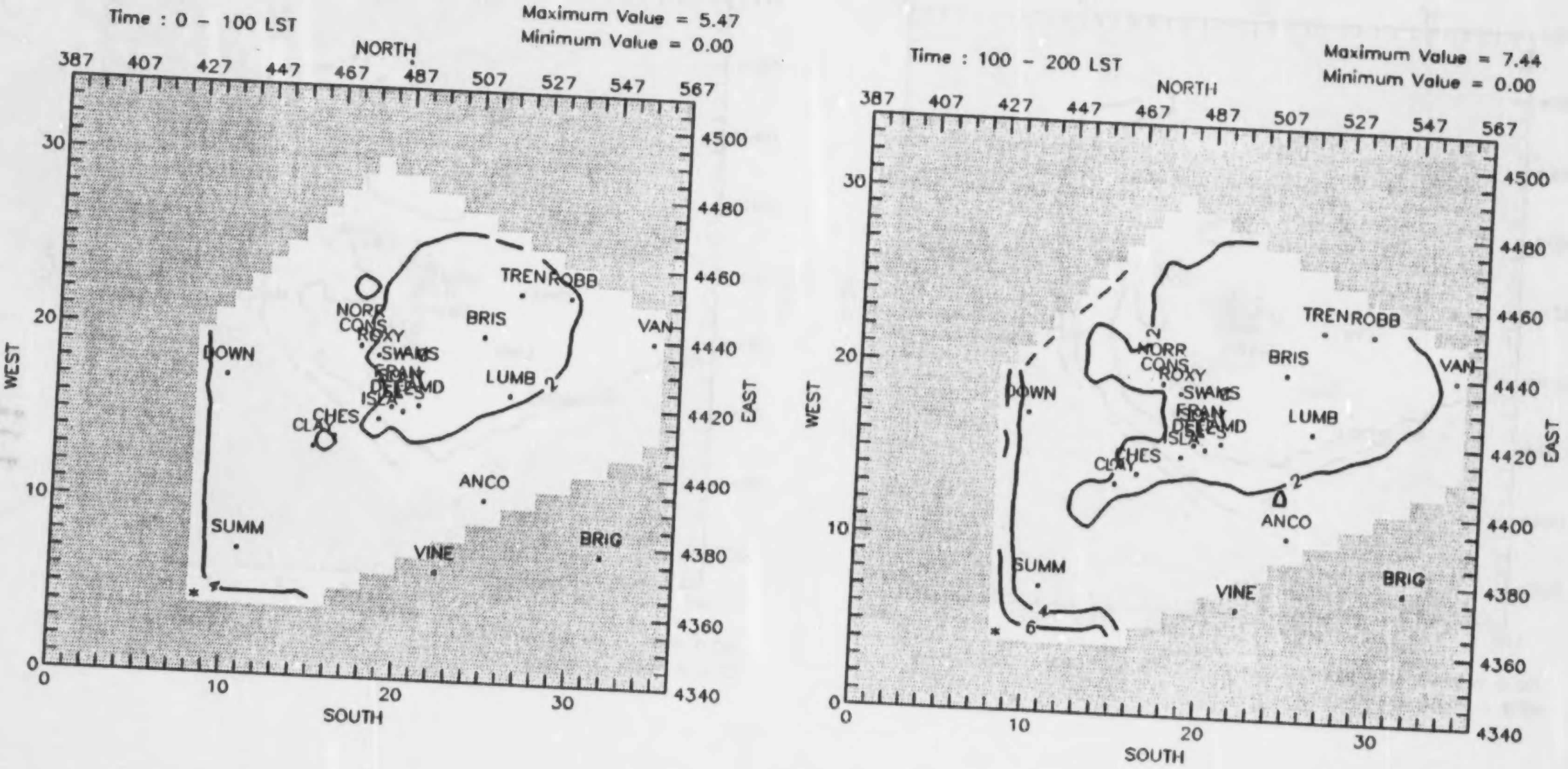
Philadelphia PLANR Winds Eval # 1
Layer 1 at hour 17 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
4490
4440
4390
4340
0
10
20
30

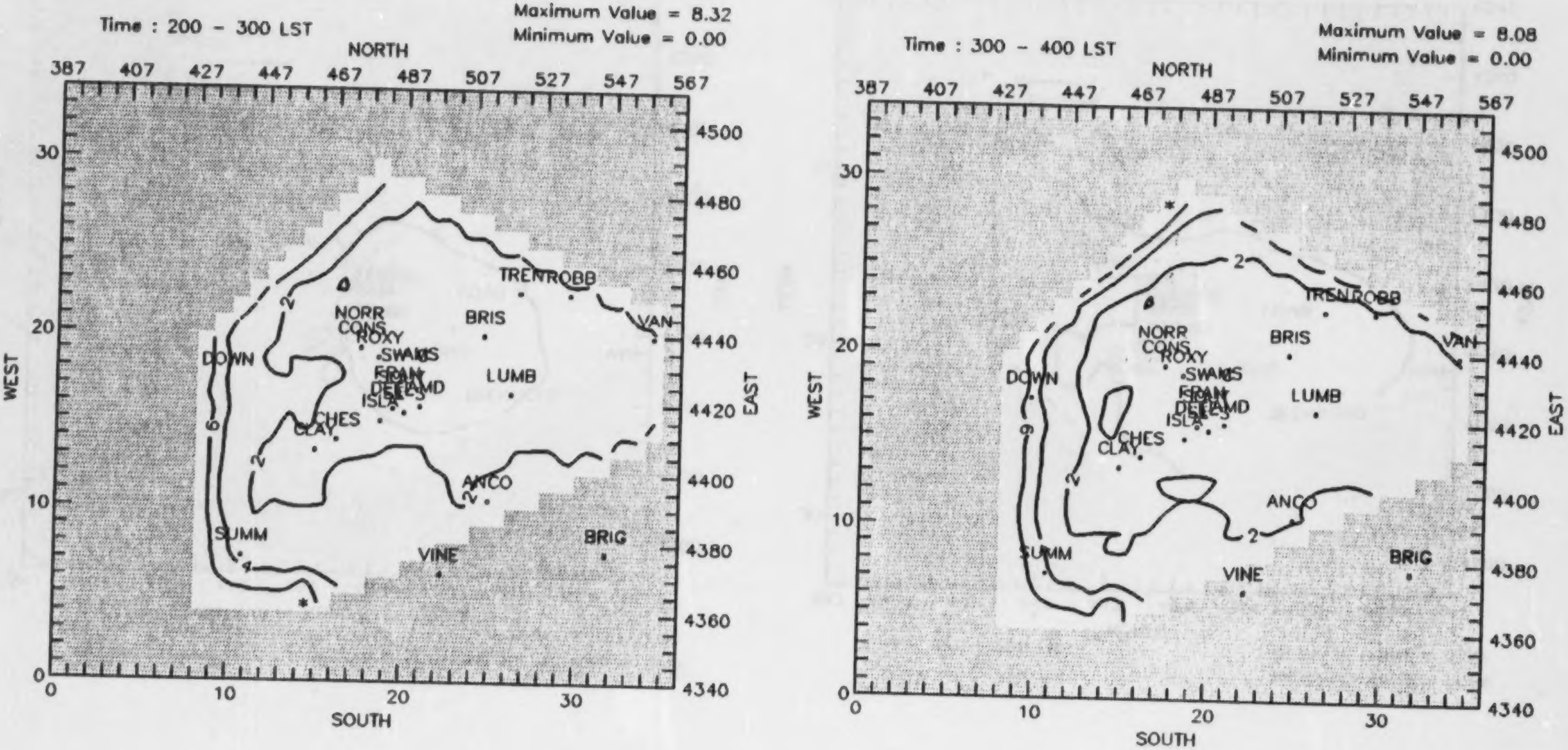
Philadelphia PLANR Winds Eval # 1
Layer 1 at hour 18 on 84194

Appendix C

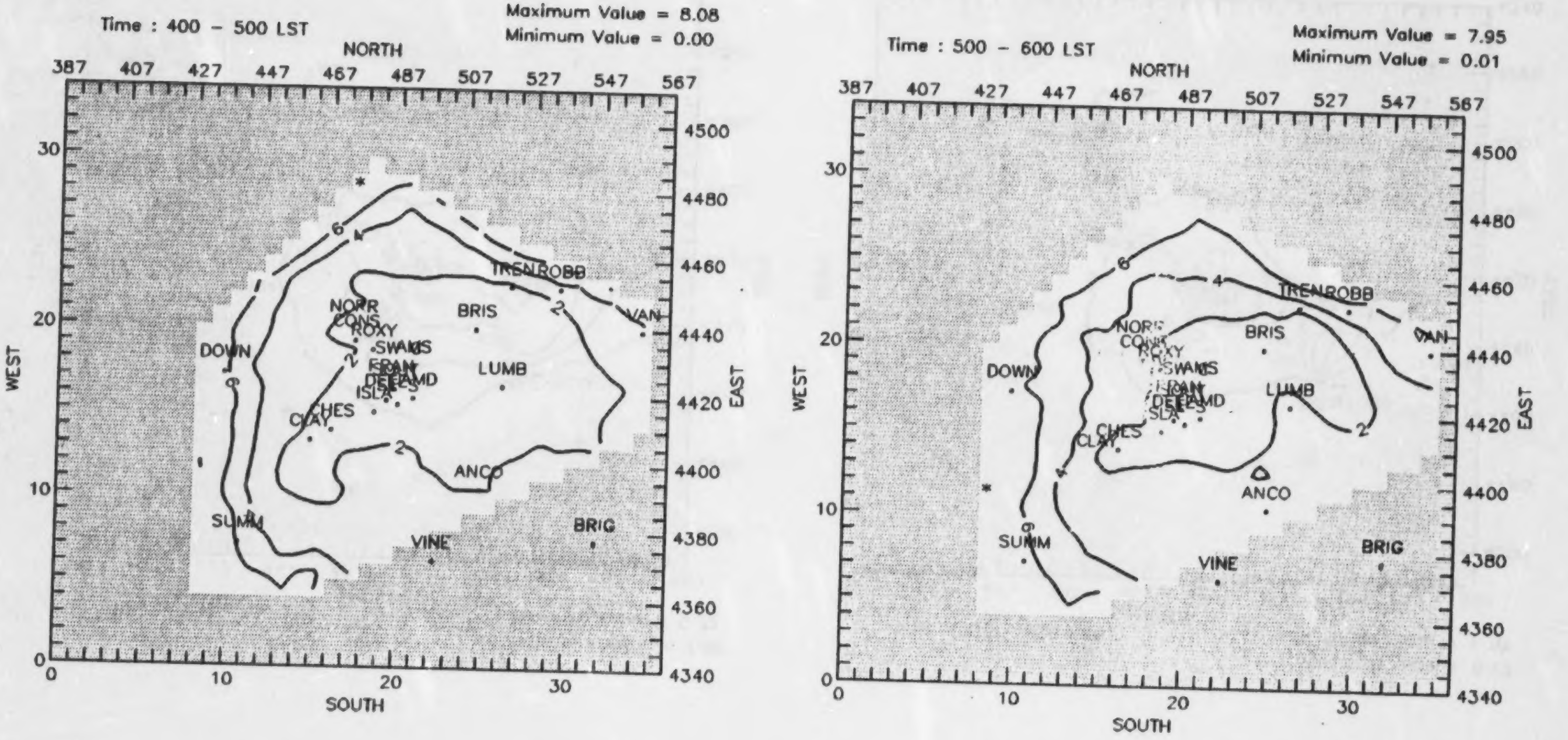
HOURLY OZONE CONCENTRATIONS (pphm) IN PHILADELPHIA PREDICTED FROM DIAGNOSTIC RUN 1


Time : 0 - 100 LST
Maximum Value = 5.47
Minimum Value = 0.00
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
0
10
20
30
4340
4360
4380
4400
4420
4440
4460
4480
4500
DOWN
SUMM
NORR
CONS
ROXY
SWAKS
FRAN
DELAMD
ISLS
CHES
CLAY
BRIS
TRENROBB
LUMB
VAN
ANCO
VINE
BRIG
2
4
Time : 100 - 200 LST
Maximum Value = 7.44
Minimum Value = 0.00
2
4
6

Ozone (pphm) 1979 base emissions, July 13, 1979


Time : 200 - 300 LST
Maximum Value = 8.32
Minimum Value = 0.00
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
DOWN
SUMM
NORR
CONS
ROXY
SWAKS
FRAN
DELAMD
ISLA
CHES
CLAY
BRIS
LUMB
TRENROBB
VAN
ANCO
VINE
BRIG
2
4
6
Time : 300 - 400 LST
Maximum Value = 8.08
Minimum Value = 0.00

Ozone (pphm) 1979 base emissions, July 13, 1979



Time : 400 - 500 LST

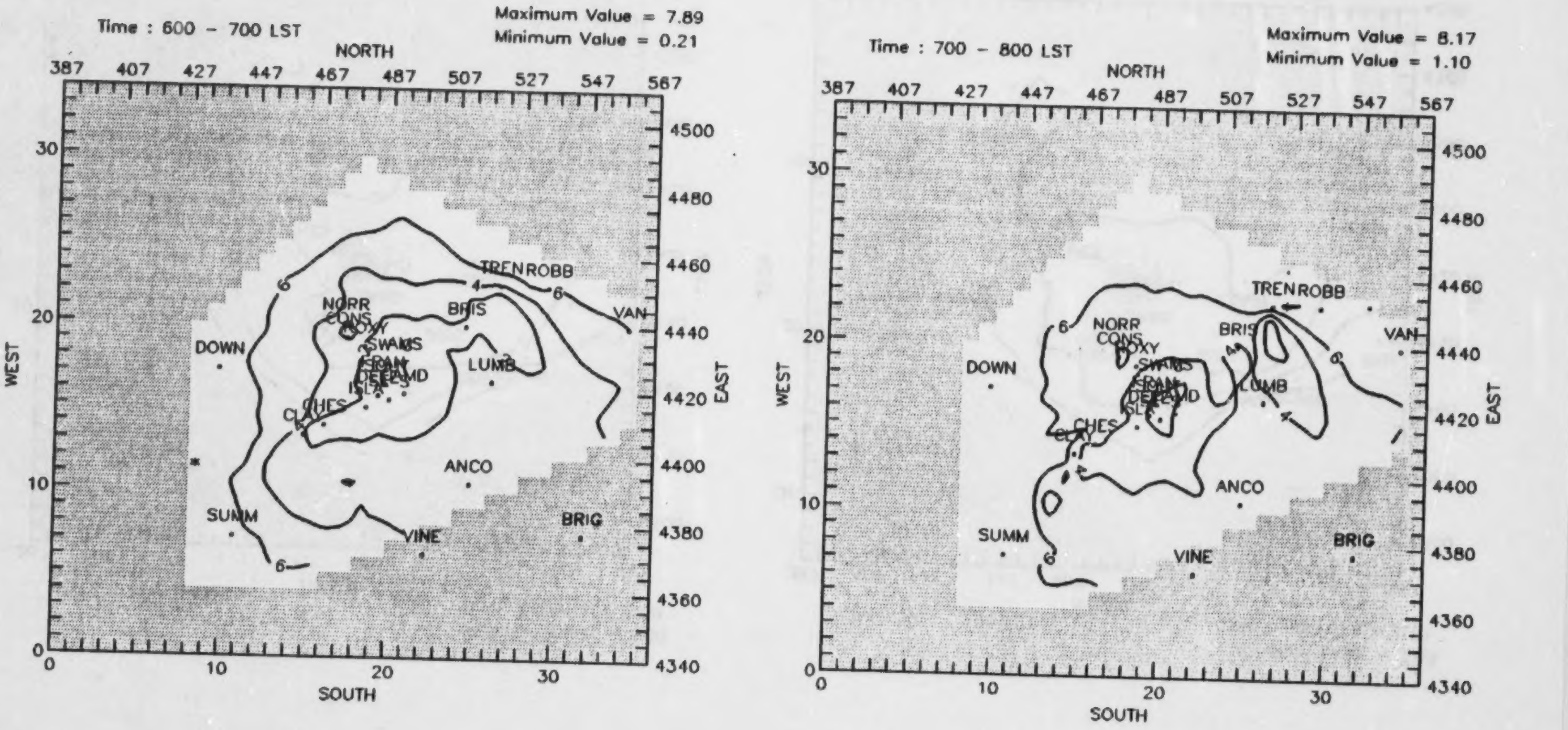
Maximum Value = 8.08
Minimum Value = 0.00

Time : 500 - 600 LST

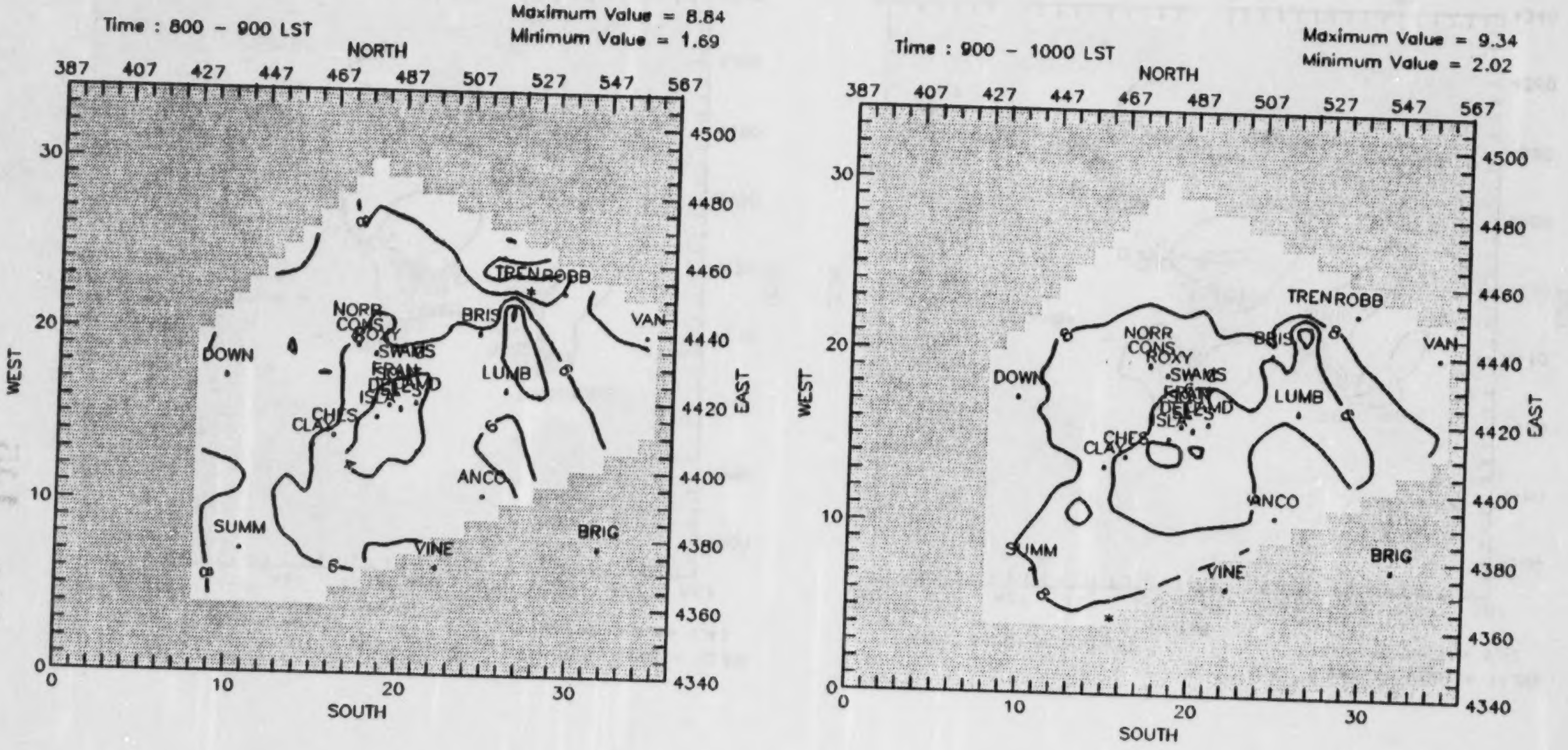
Maximum Value = 7.95
Minimum Value = 0.01

NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
DOWN
SUMM
NORR
CONS
ROXY
SWANS
FRAN
DEEAMD
ISLA
CHES
CLAY
BRIS
LUMB
TRENROBB
VAN
ANCO
VINE
BRIG
2
4
6

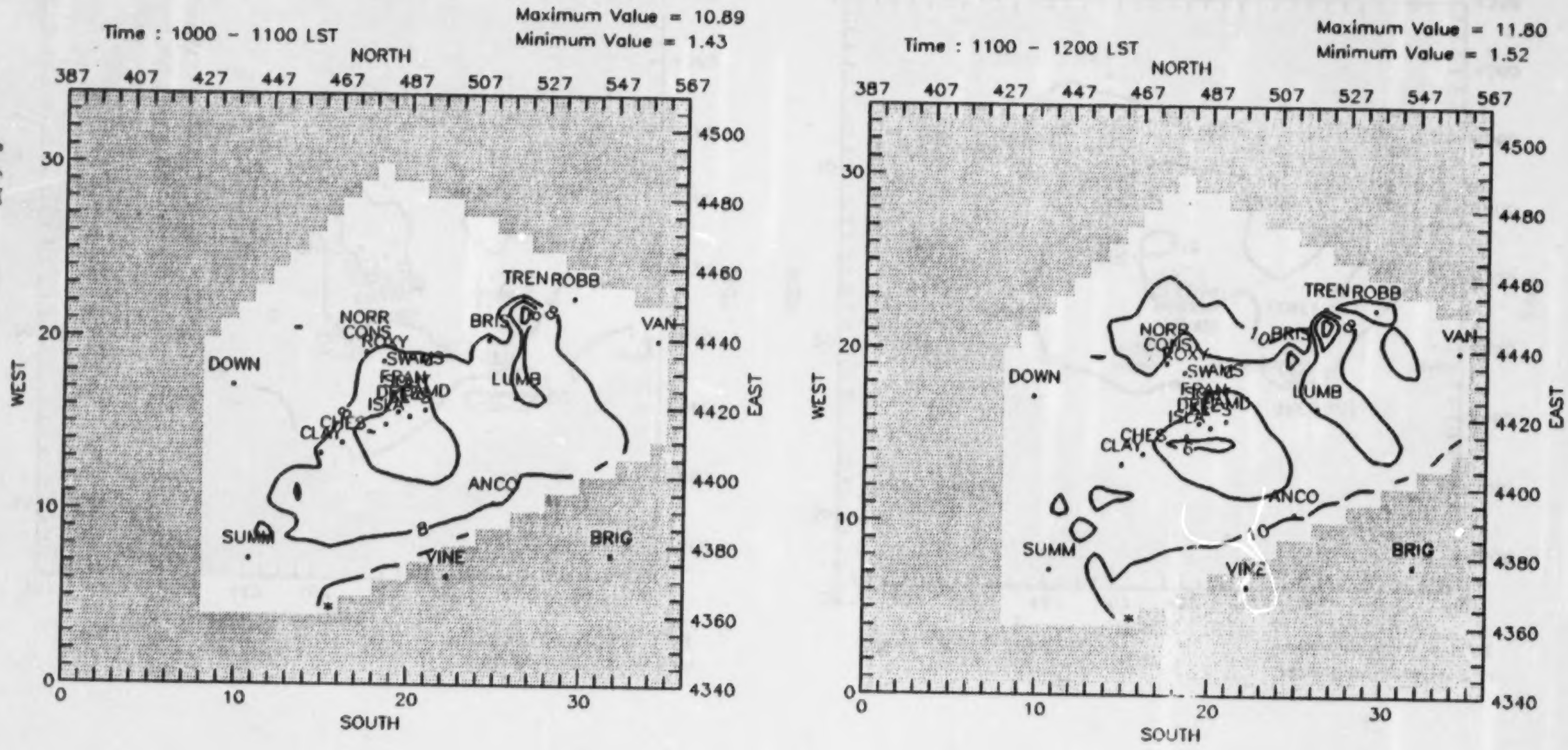
Ozone (pphm) 1979 base emissions, July 13, 1979


Time : 600 - 700 LST
Maximum Value = 7.89
Minimum Value = 0.21
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
VAN
NORR
CONS
OXY
SWANS
FRAN
DELE
ISLA
LAMD
BRIS
LUMB
DOWN
CHES
CLAY
ANCO
SUMM
VINE
BRIG
4
6
Time : 700 - 800 LST
Maximum Value = 8.17
Minimum Value = 1.10

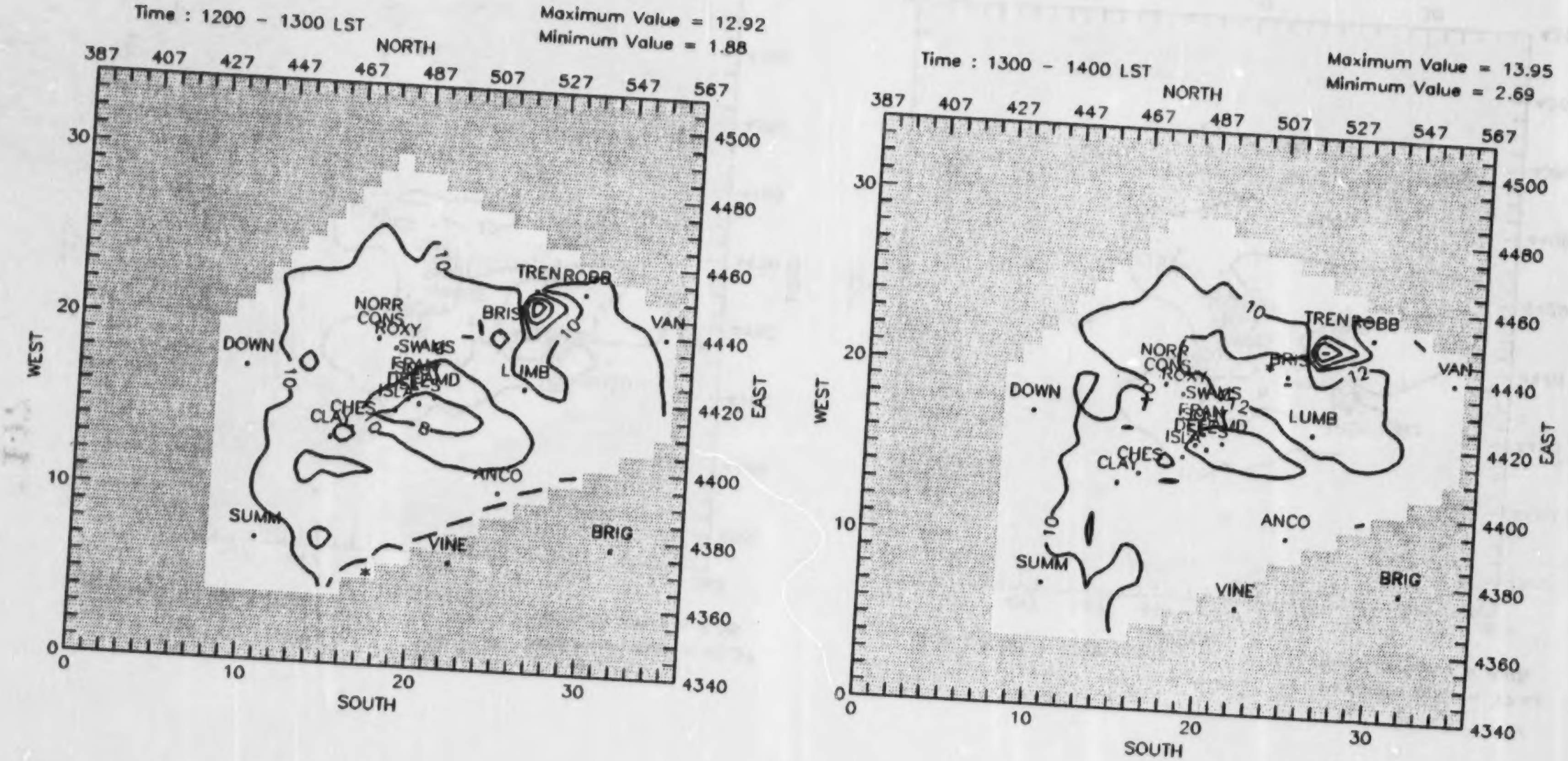
Ozone (pphm) 1979 base emissions, July 13, 1979


Time : 800 - 900 LST
Maximum Value = 8.84
Minimum Value = 1.69
Time : 900 - 1000 LST
Maximum Value = 9.34
Minimum Value = 2.02
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
NORR
CONS
ROXY
SWANS
FRAN
DELAMD
ISLES
CHES
CLAY
BRIS
LUMB
ANCO
DOWN
SUMM
VINE
BRIG
VAN
6
8

Ozone (pphm) 1979 base emissions, July 13, 1979

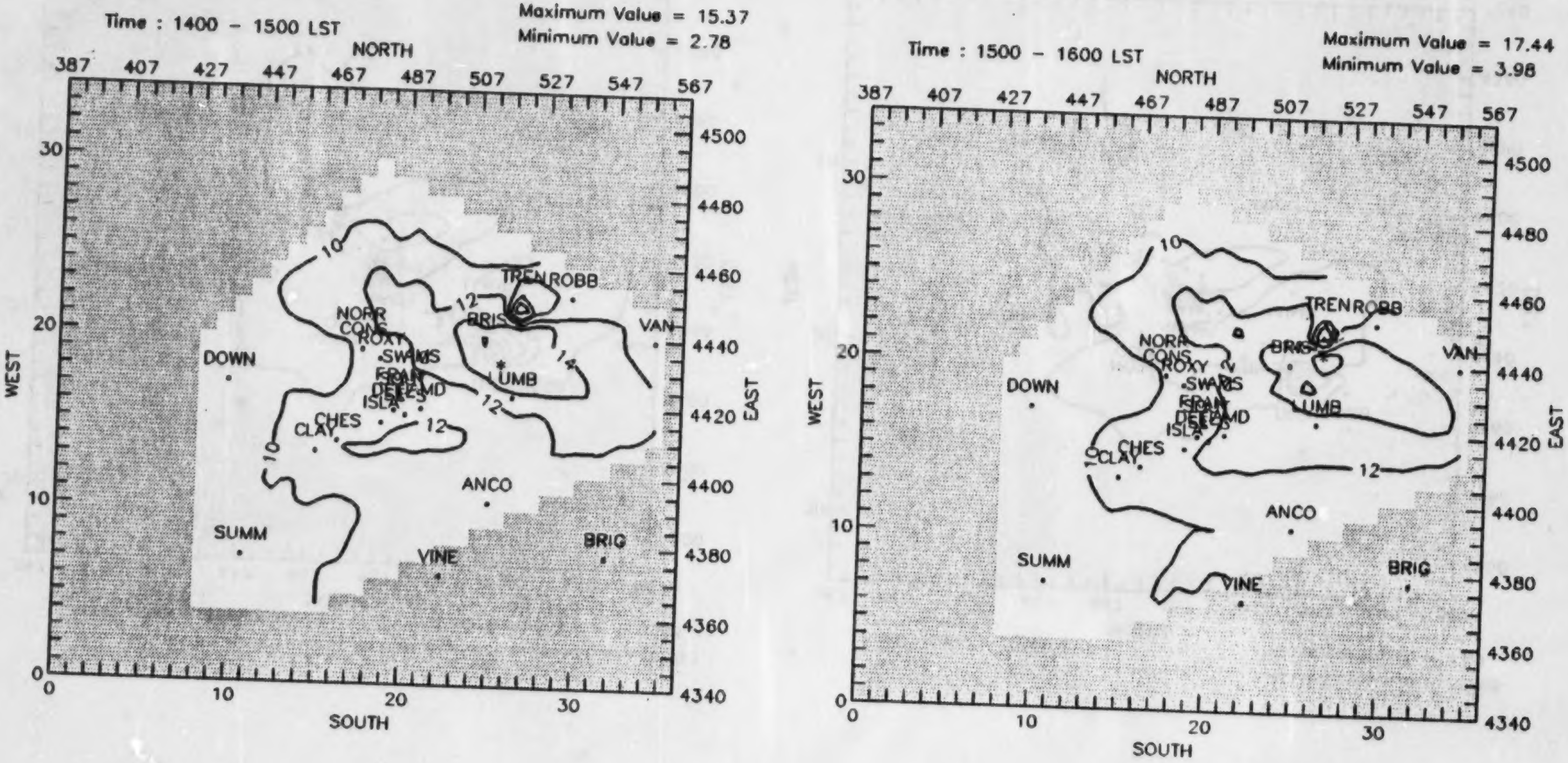

Time : 1000 - 1100 LST
Maximum Value = 10.89
Minimum Value = 1.43
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
DOWN
NORR
CONS
ROXY
SWANS
FRAN
DREAMD
ISLE
CHES
CLAY
SUMM
TREN
ROBB
BRIS
LUMB
VAN
ANCO
VINE
BRIG
8
Time : 1100 - 1200 LST
Maximum Value = 11.80
Minimum Value = 1.52
10
6

Ozone (pphm) 1979 base emissions, July 13, 1979

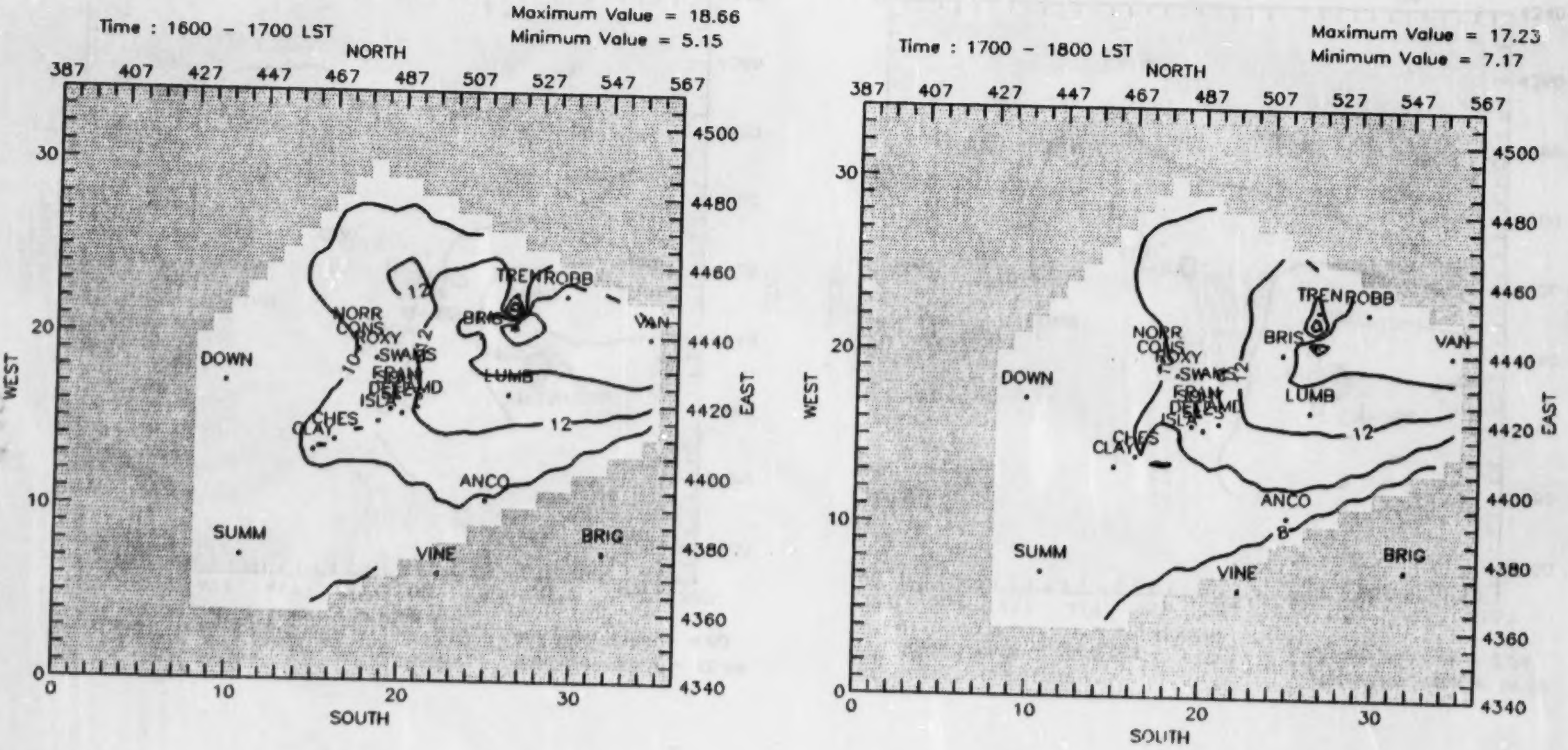


Time : 1200 - 1300 LST
Maximum Value = 12.92
Minimum Value = 1.88
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TREN
ROBB
BRIS
VAN
NORR
CONS
ROXY
SWANS
FRAN
DEFAMD
ISLES
CHES
CLAY
DOWN
LUMB
ANCO
SUMM
VINE
BRIG
8
10
Time : 1300 - 1400 LST
Maximum Value = 13.95
Minimum Value = 2.69
12

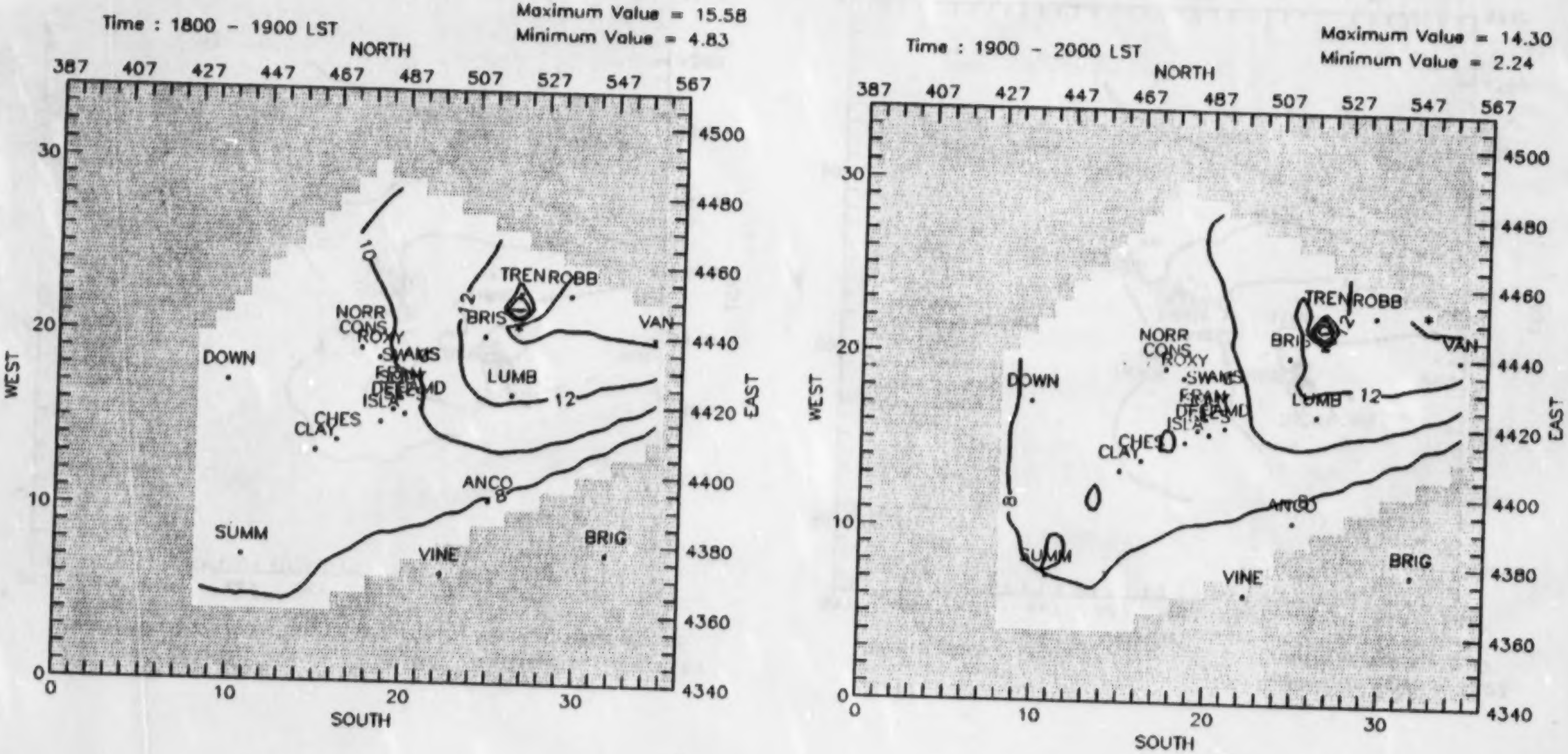
Ozone (pphm) 1979 base emissions, July 13, 1979


Time : 1400 - 1500 LST
Maximum Value = 15.37
Minimum Value = 2.78
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
BRIS
VAN
NORR
CONS
ROXY
SWAMS
FRAN
DELEMD
ISLA
CHES
CLAY
DOWN
LUMB
ANCO
SUMM
VINE
BRIG
10
12
14
Time : 1500 - 1600 LST
Maximum Value = 17.44
Minimum Value = 3.98

Ozone (pphm) 1979 base emissions, July 13, 1979


Time : 1600 - 1700 LST
Maximum Value = 18.66
Minimum Value = 5.15
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
NORR
CONS
ROXY
SWARS
FRAN
DELEAMD
ISLA
BRIS
VAN
LUMB
CHES
CLAY
DOWN
ANCO
SUMM
VINE
BRIG
12
10
Time : 1700 - 1800 LST
Maximum Value = 17.23
Minimum Value = 7.17
8

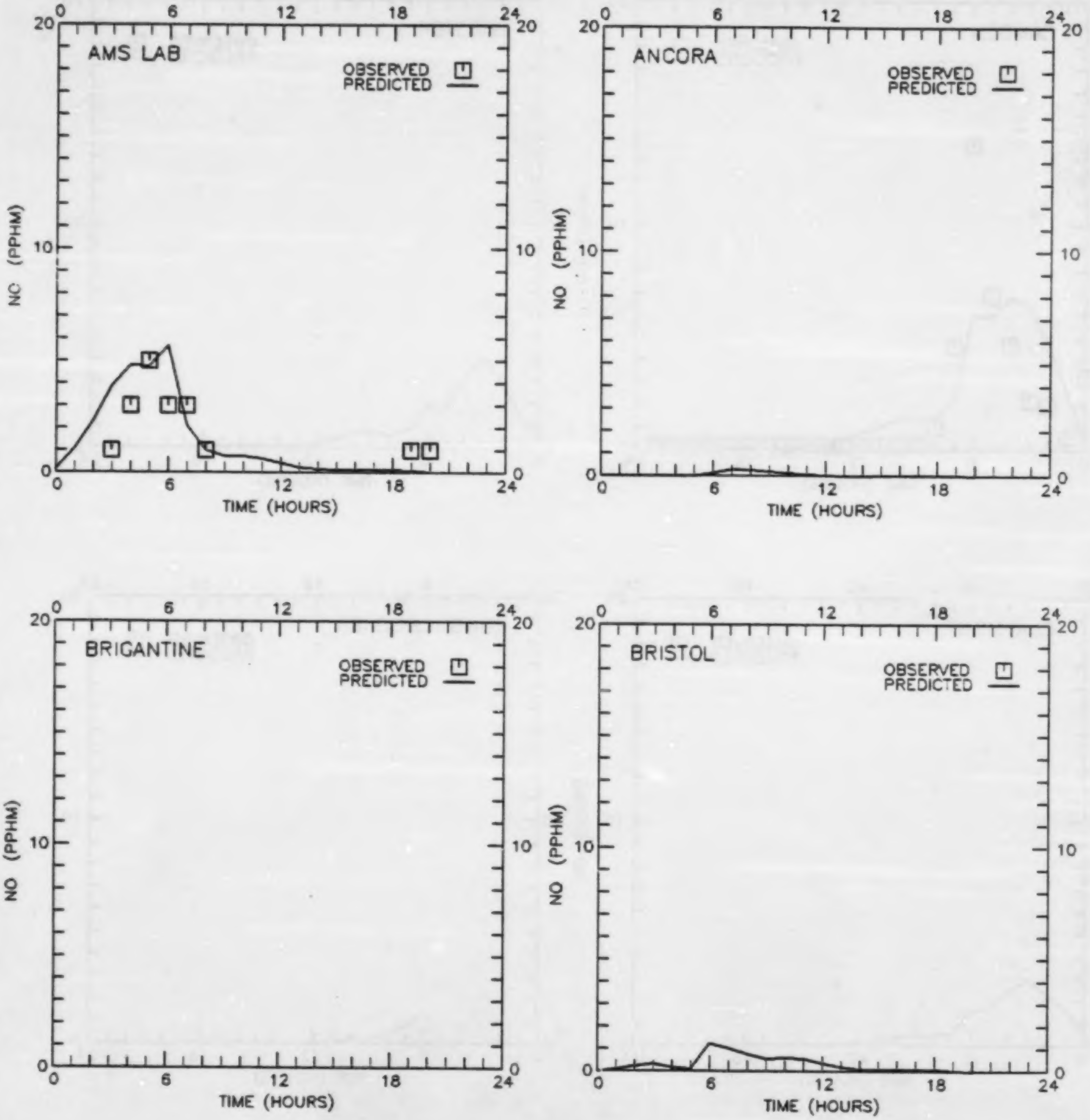
Ozone (pphm) 1979 base emissions, July 13, 1979


Time : 1800 - 1900 LST
Maximum Value = 15.58
Minimum Value = 4.83
NORTH
387
407
427
447
467
487
507
527
547
567
WEST
EAST
SOUTH
0
10
20
30
4340
4360
4380
4400
4420
4440
4460
4480
4500
DOWN
NORR
CONS
ROXY
SWANS
FRAN
DEL
FERMD
ISLA
CHES
CLAY
TREN
ROBB
BRIS
VAN
LUMB
ANCO
SUMM
VINE
BRIG
10
12
8
Time : 1900 - 2000 LST
Maximum Value = 14.30
Minimum Value = 2.24
NORTH
387
407
427
447
467
487
507
527
547
567
WEST
EAST
SOUTH
0
10
20
30
4340
4360
4380
4400
4420
4440
4460
4480
4500
DOWN
NORR
CONS
ROXY
SWANS
FRAN
DEL
FERMD
ISLA
CHES
CLAY
TREN
ROBB
BRIS
VAN
LUMB
ANCO
SUMM
VINE
BRIG
12
8

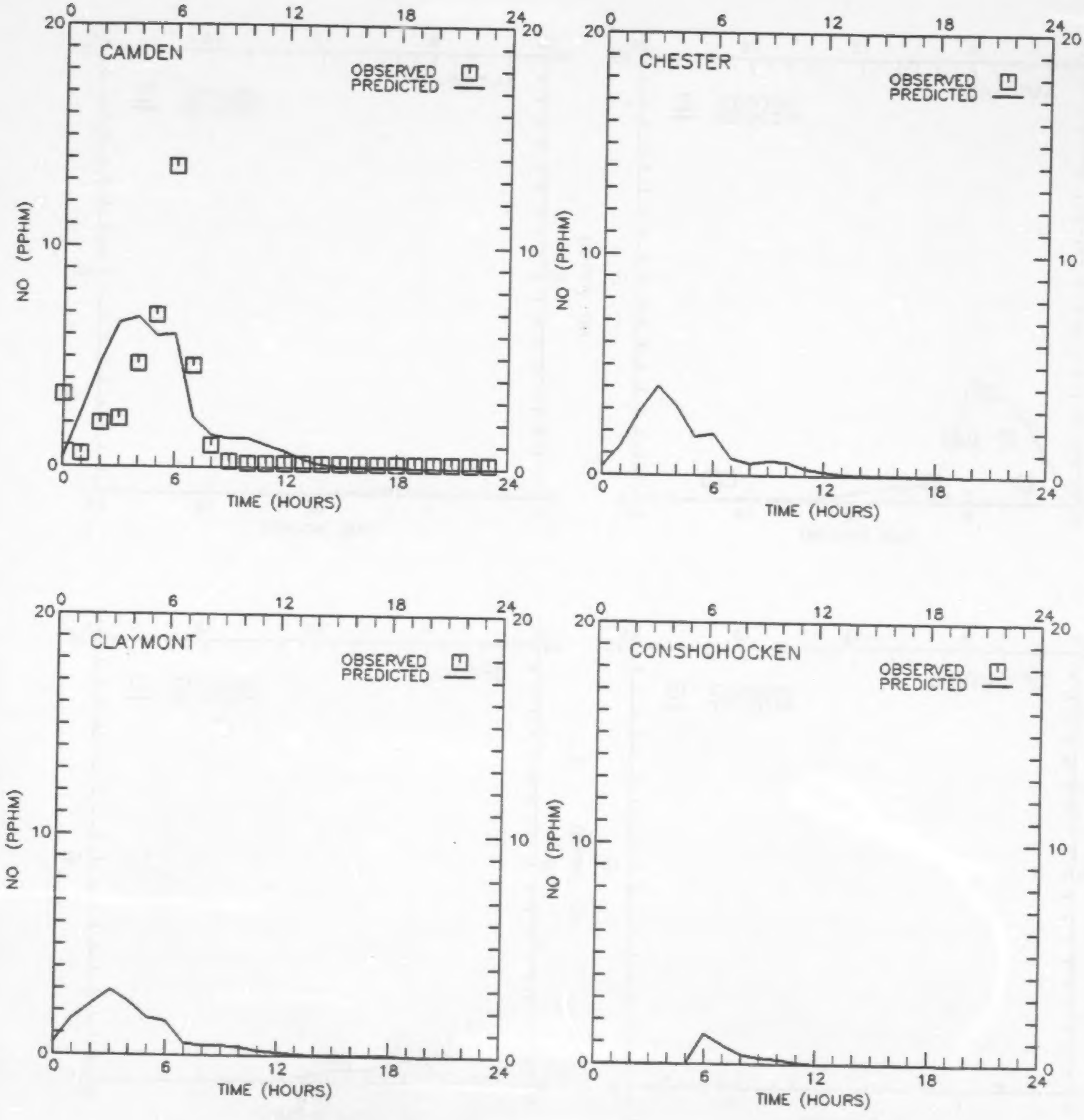
Ozone (pphm) 1979 base emissions, July 13, 1979

Appendix D

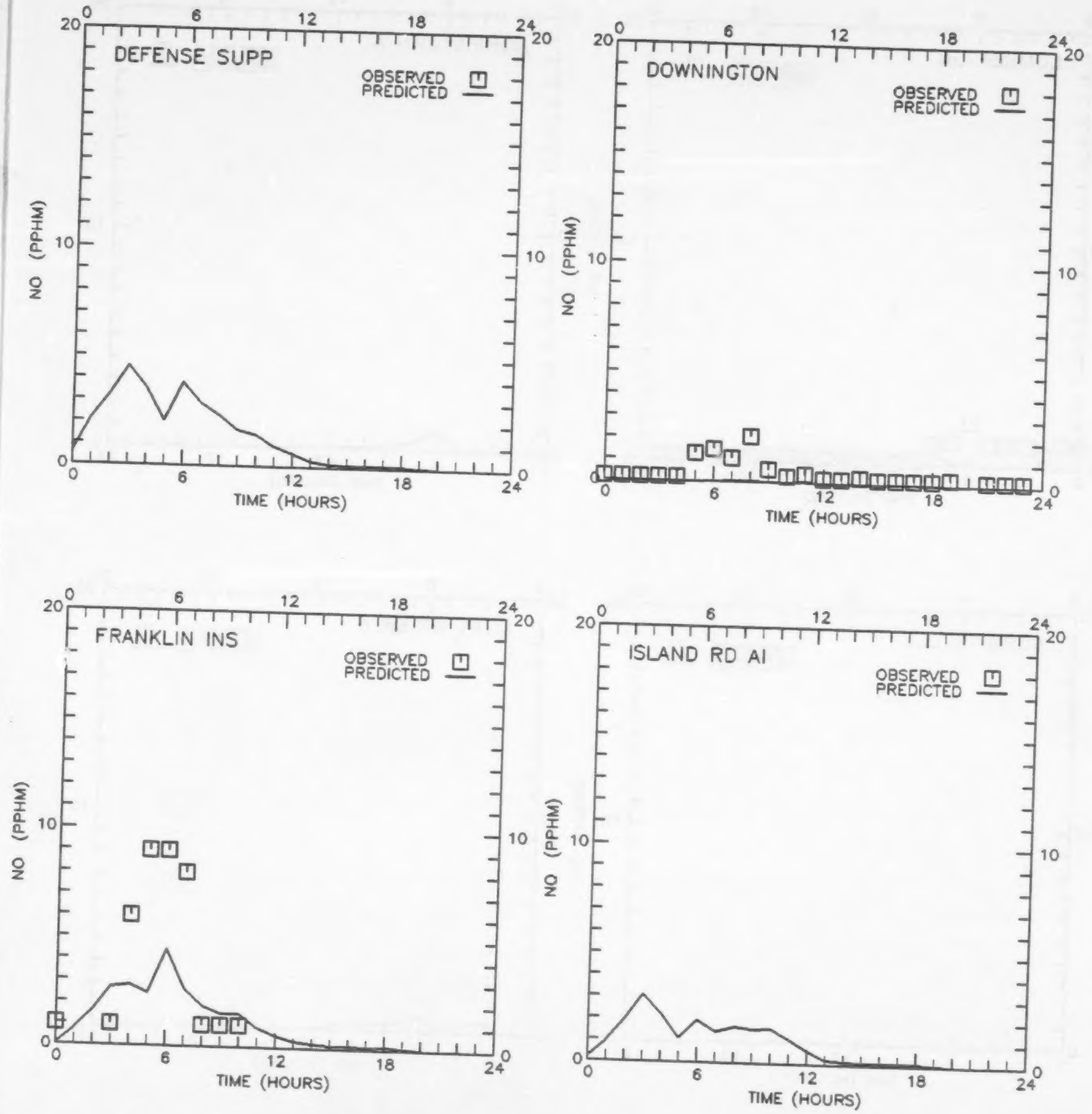
TIME SERIES OF PREDICTED AND OBSERVED HOURLY NO, NO_2, AND CO CONCENTRATIONS IN PHILADELPHIA FOR DIAGNOSTIC RUN 1



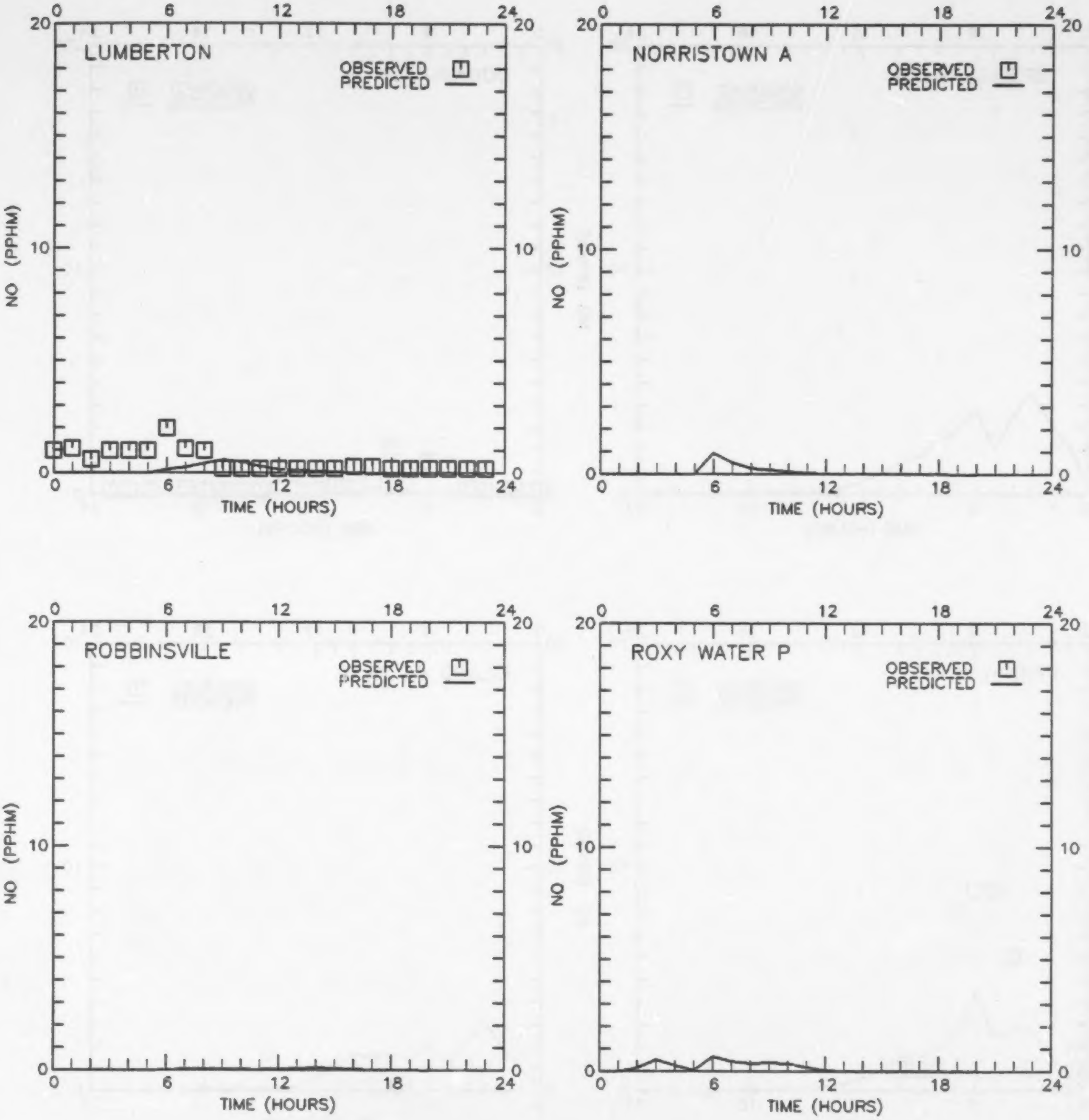
PHILADELPHIA – 7/13/79 – NO – PLANR RUN #1



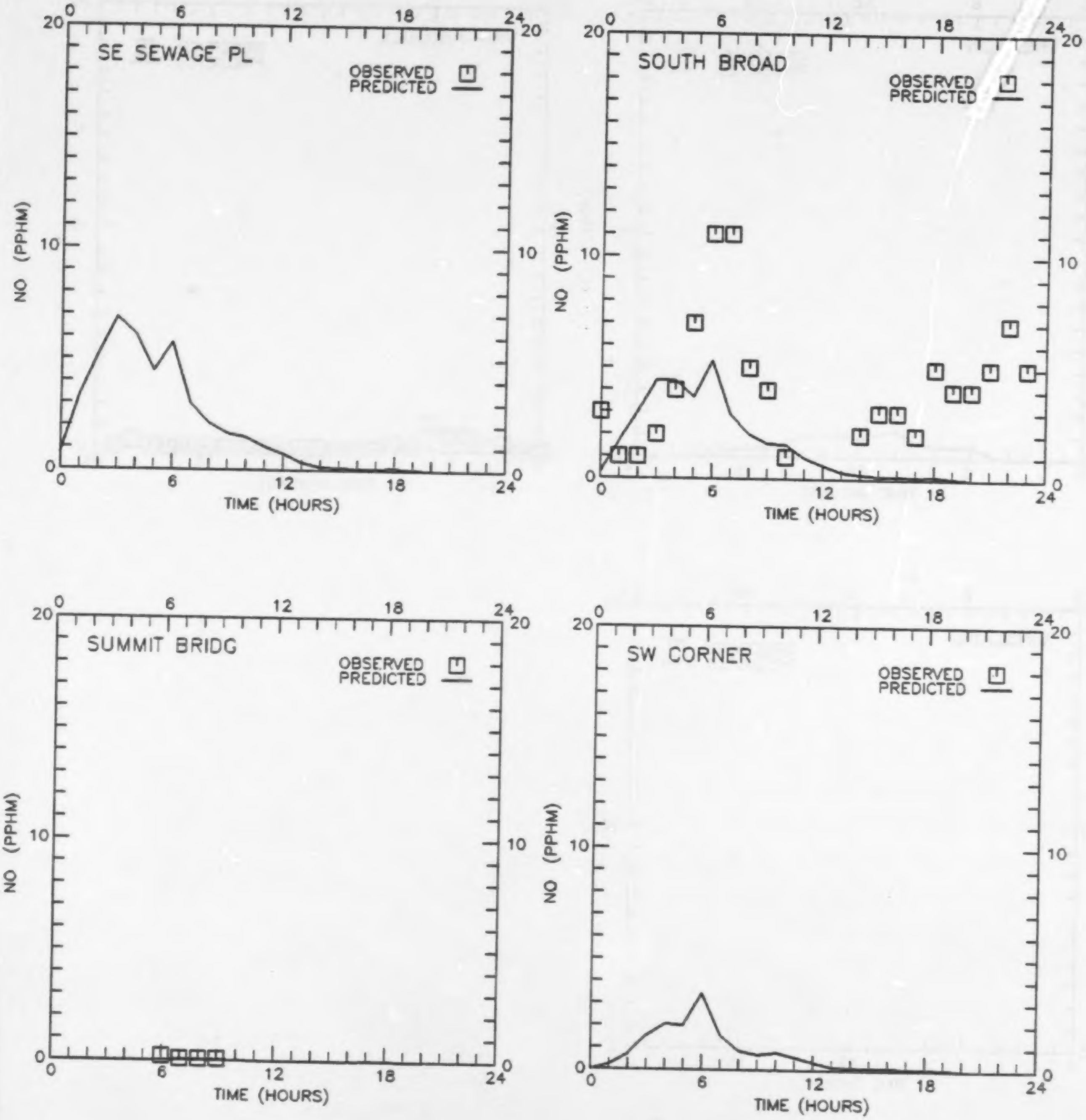
PHILADELPHIA – 7/13/79 – NO – PLANR RUN #1



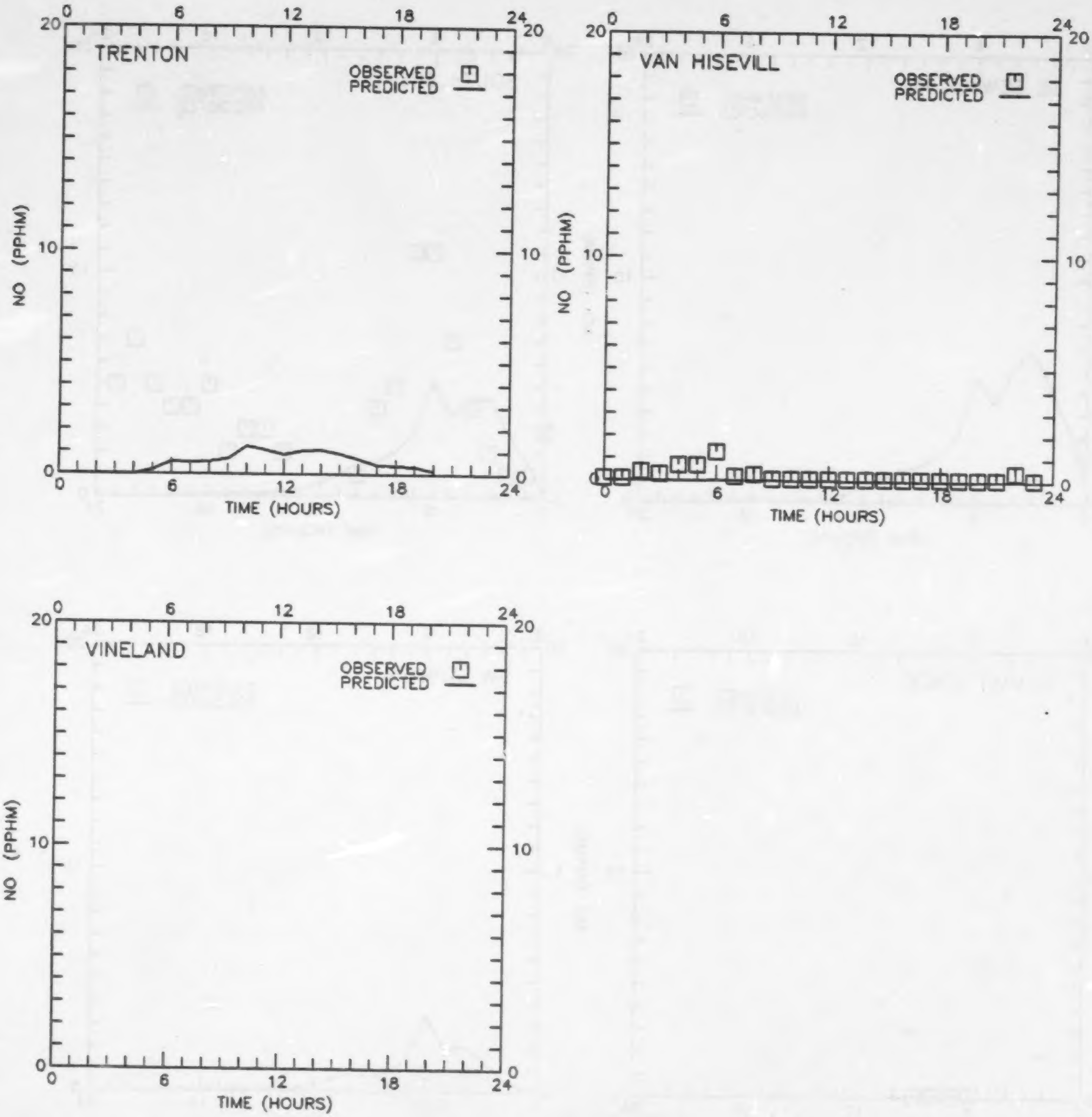
PHILADELPHIA – 7/13/79 – NO – PLANR RUN #1



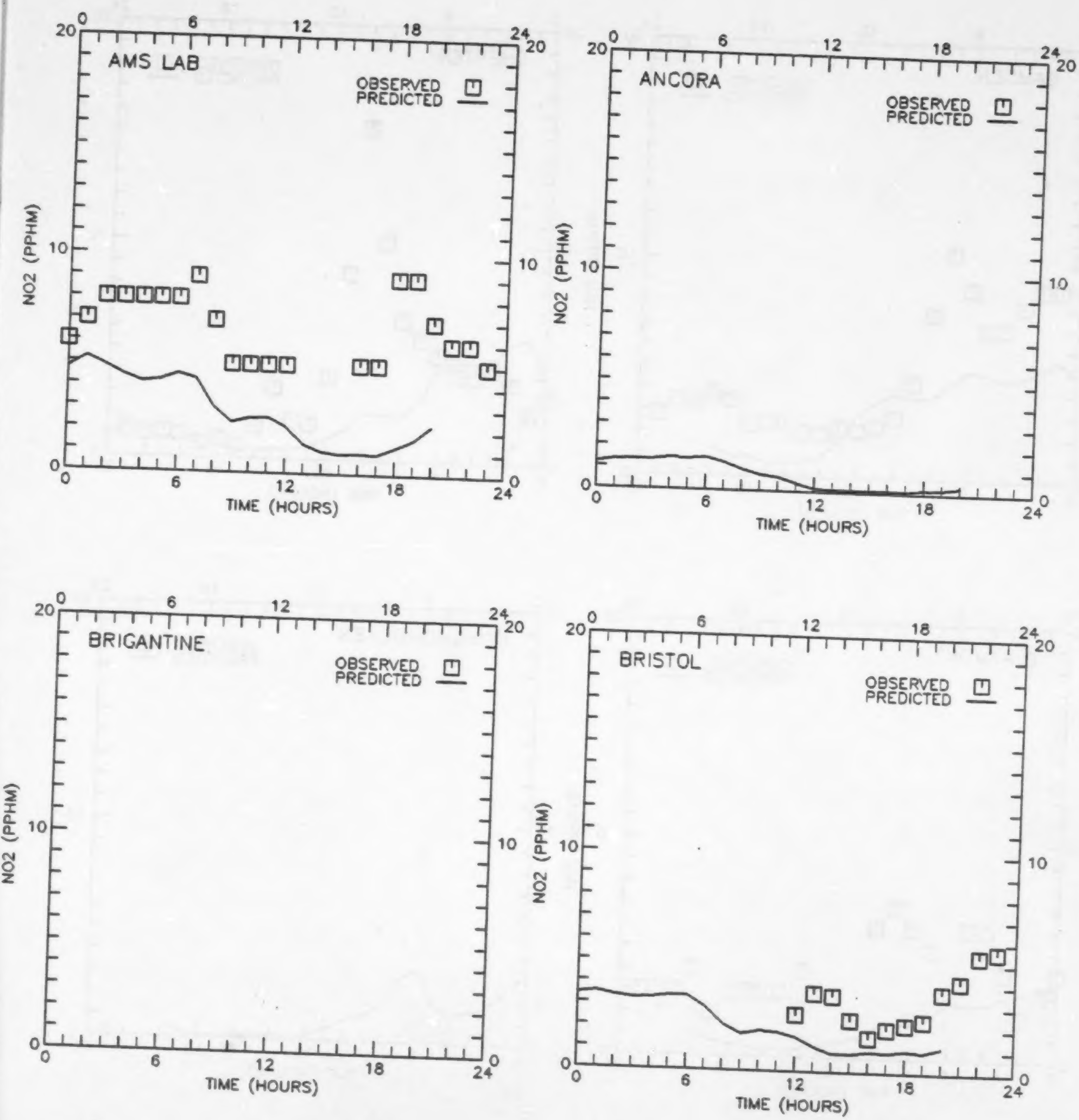
PHILADELPHIA – 7/13/79 – NO – PLANR RUN #1



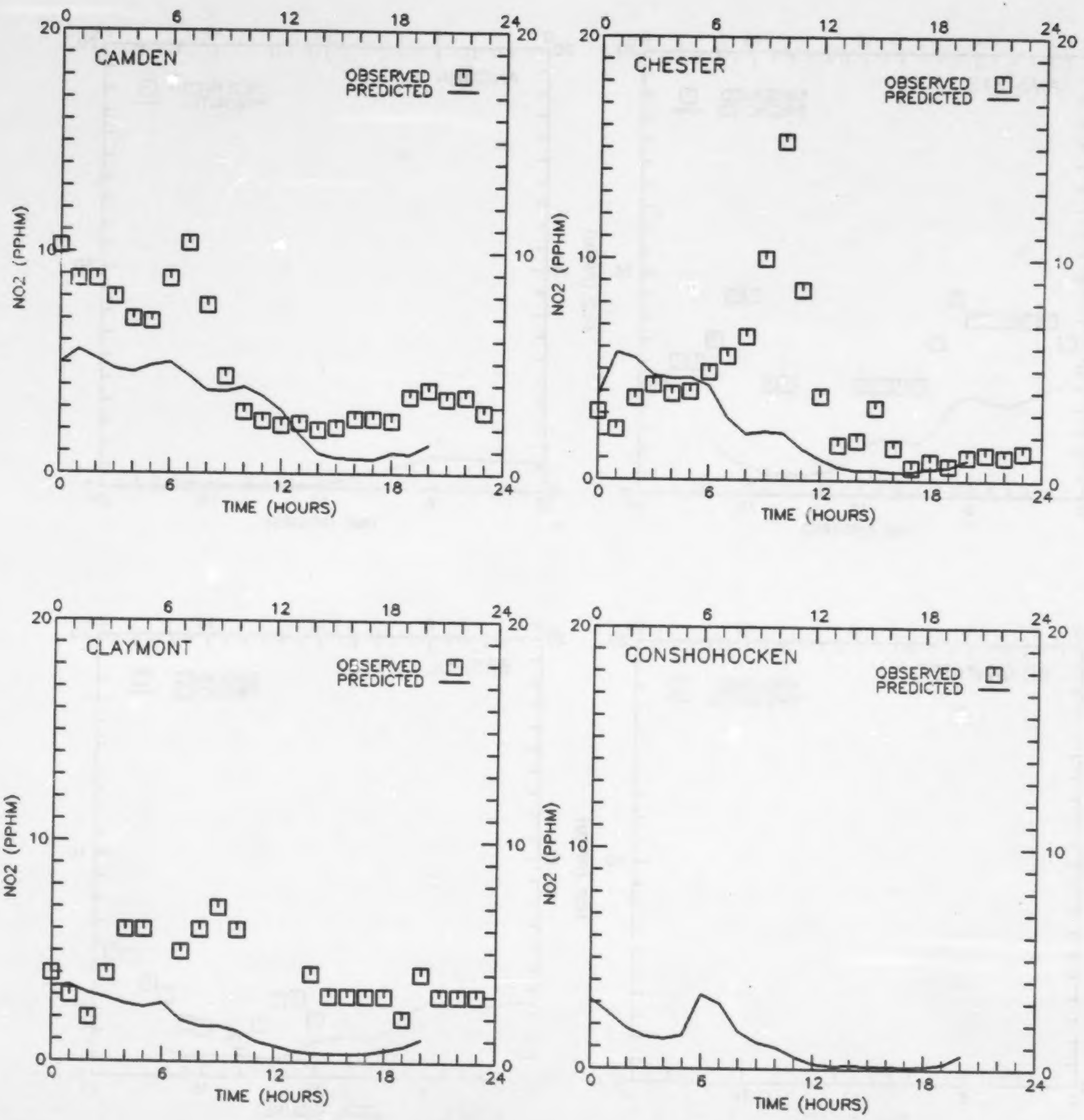
PHILADELPHIA – 7/13/79 – NO – PLANR RUN #1



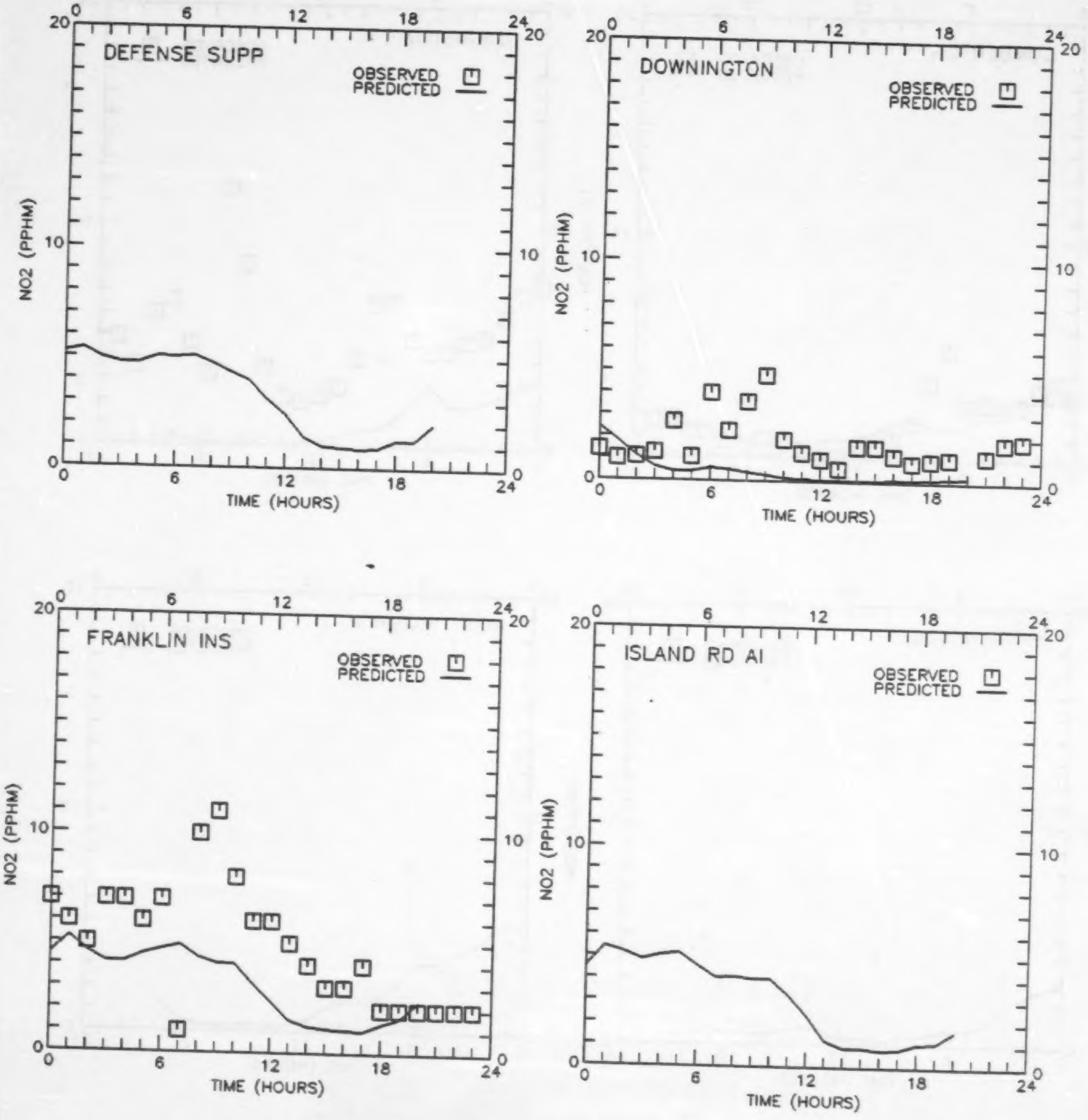
PHILADELPHIA – 7/13/79 – NO – PLANR RUN #1



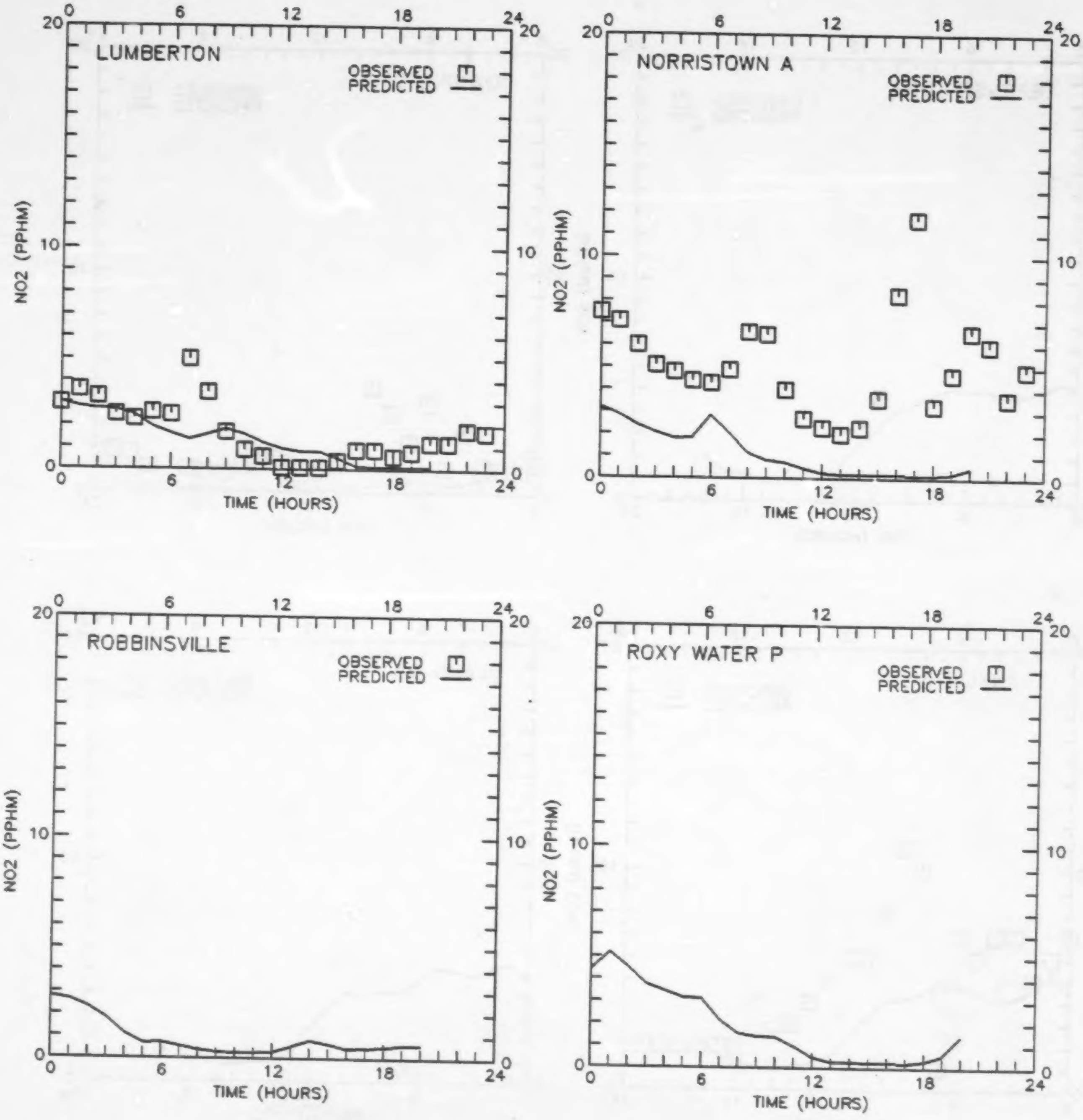
PHILADELPHIA – 7/13/79 – NO2 – PLANR RUN #1



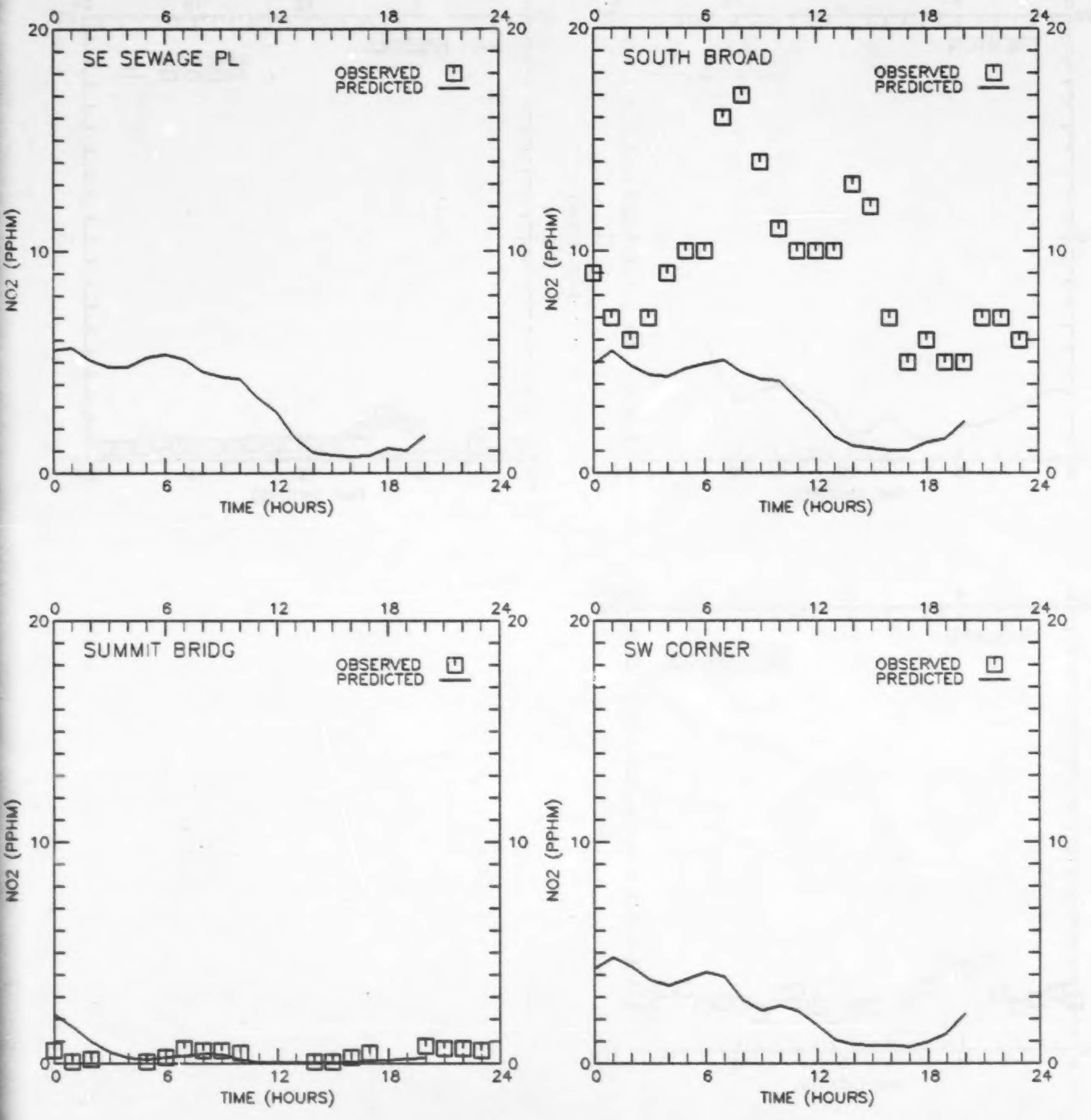
PHILADELPHIA – 7/13/79 – NO2 – PLANR RUN #1



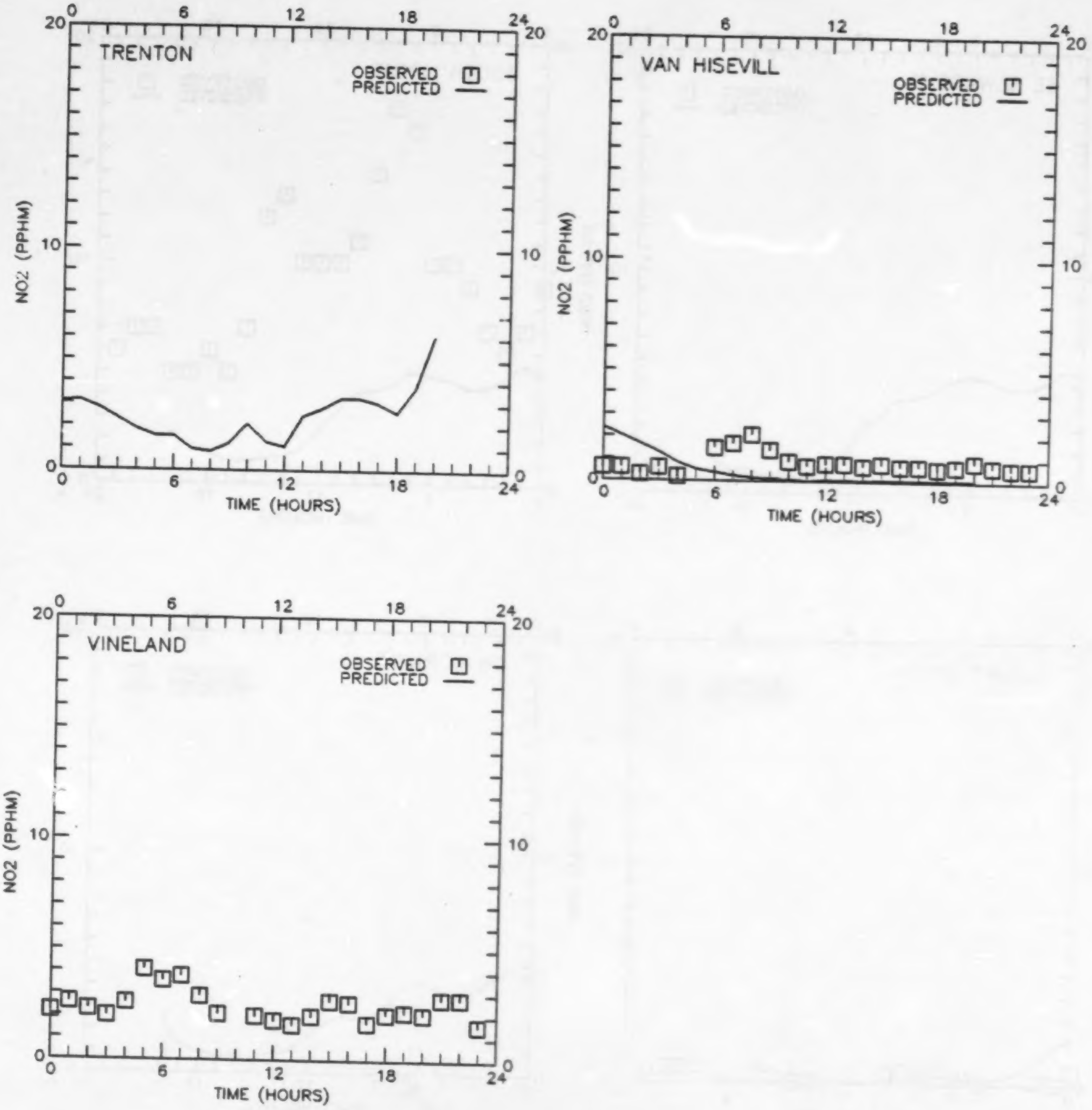
PHILADELPHIA – 7/13/79 – NO2 – PLANR RUN #1



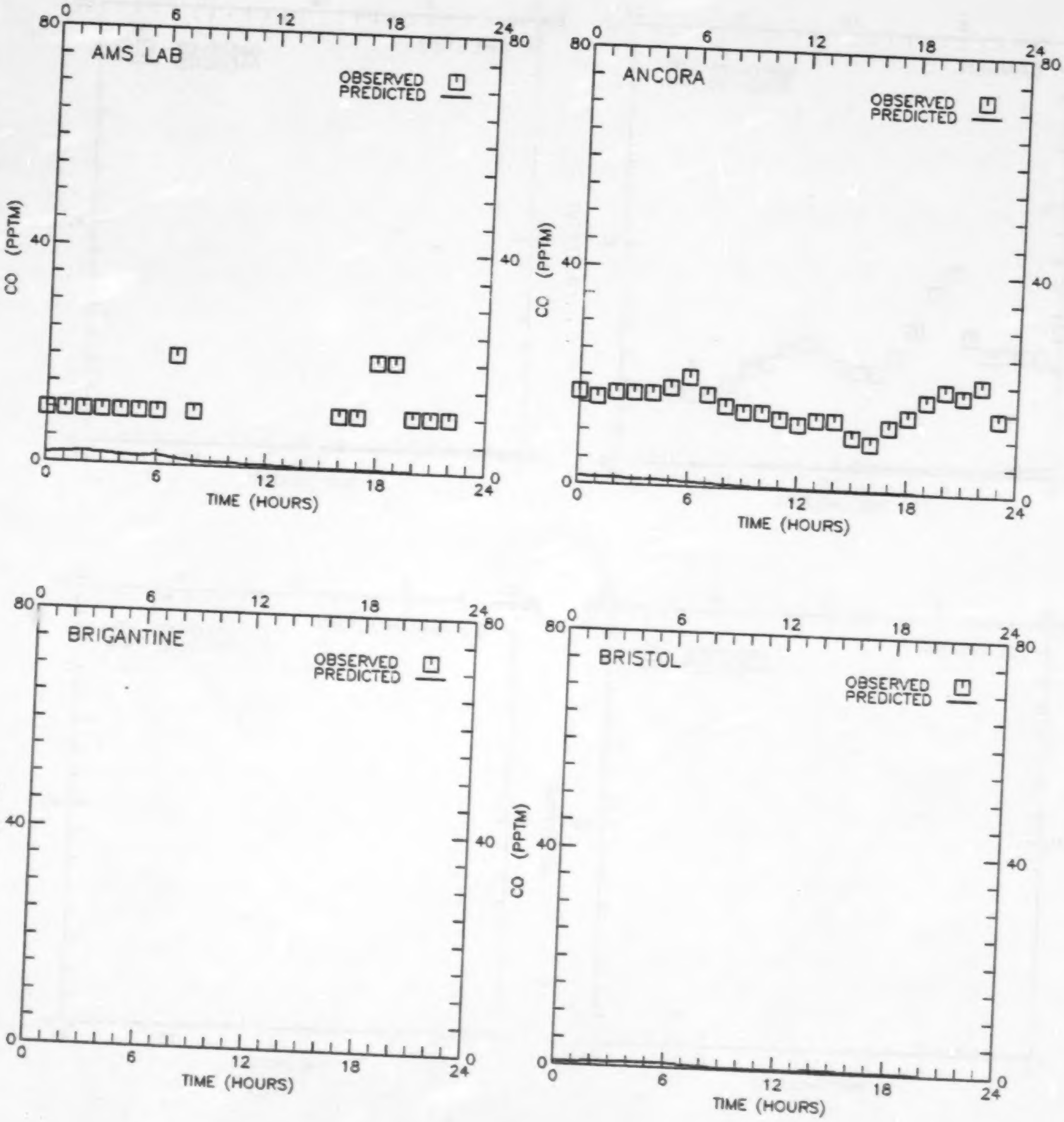
PHILADELPHIA – 7/13/79 – NO2 – PLANR RUN #1



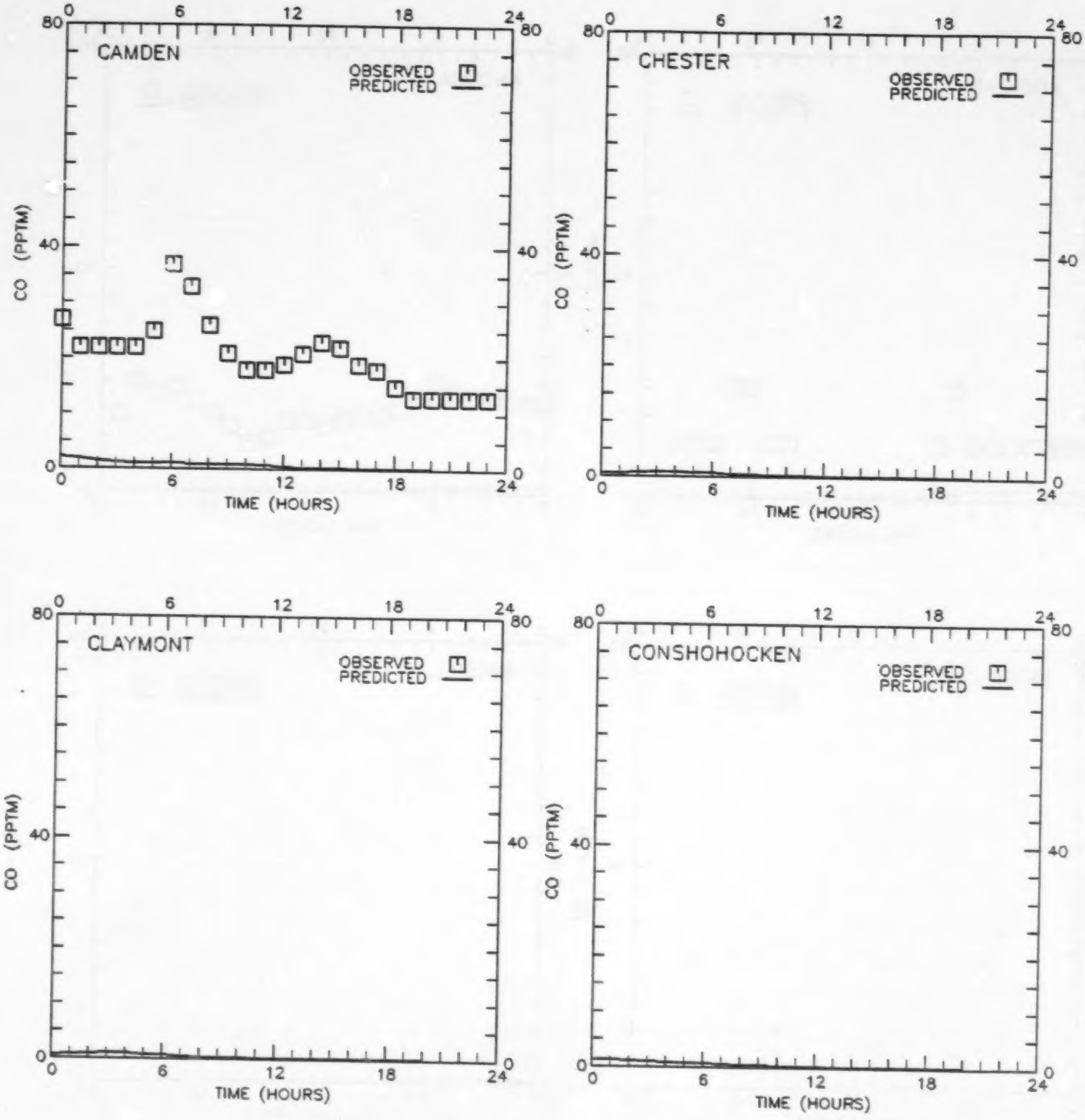
PHILADELPHIA – 7/13/79 – NO2 – PLANR RUN #1



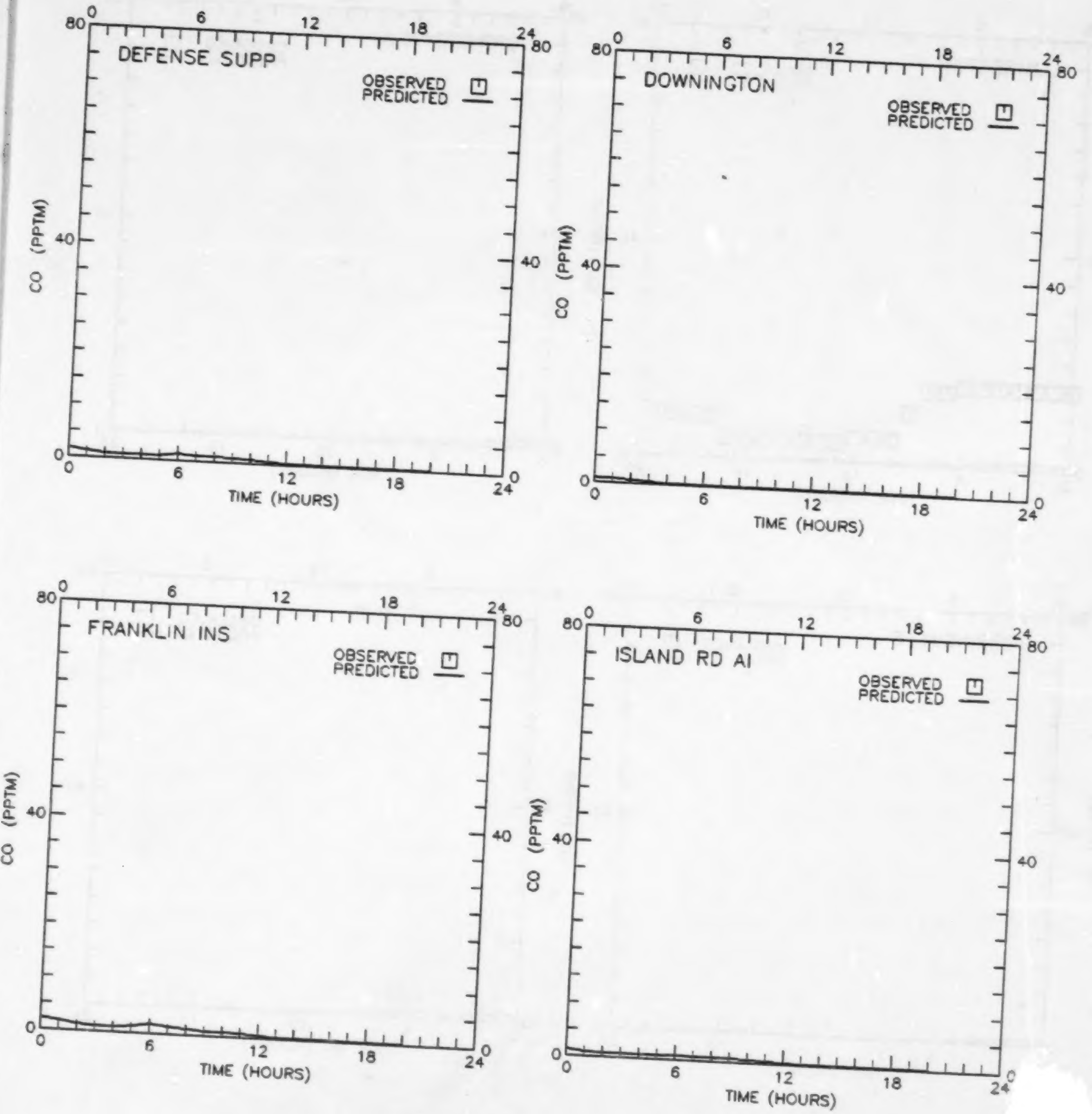
PHILADELPHIA – 7/13/79 – NO2 – PLANR RUN #1



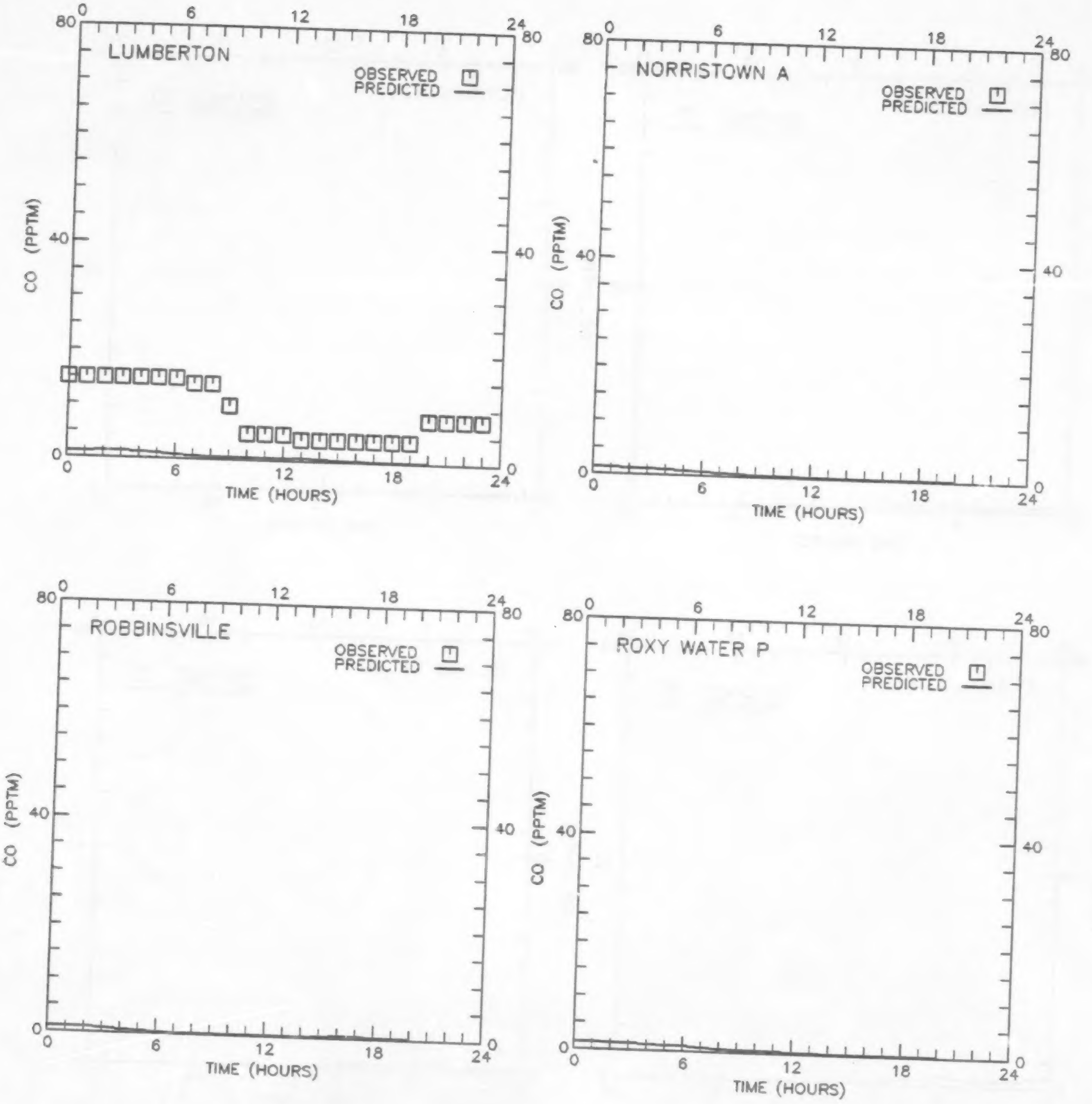
PHILADELPHIA – 7/13/79 – CO – PLANR RUN #1



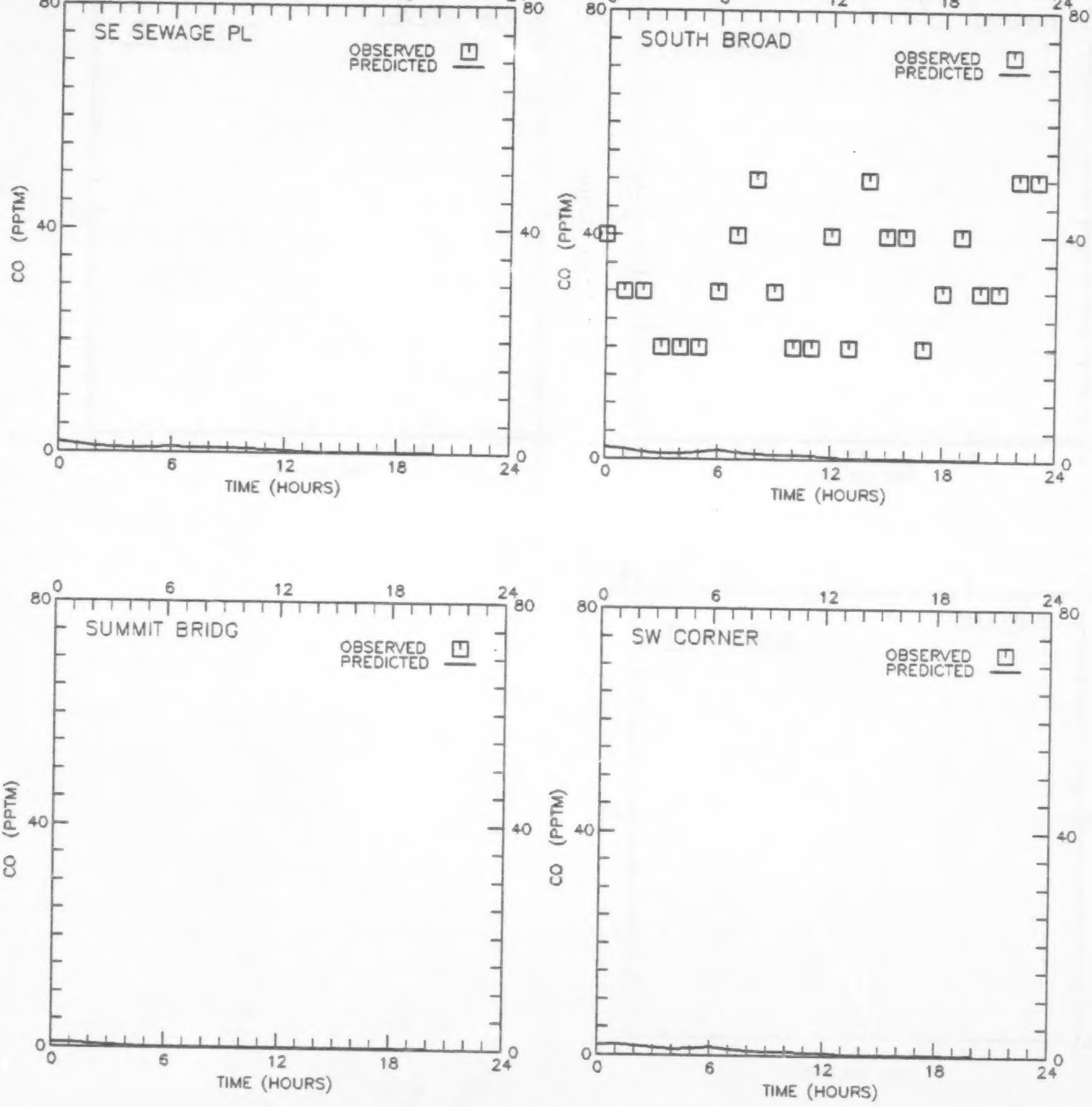
PHILADELPHIA – 7/13/79 – CO – PLANR RUN #1



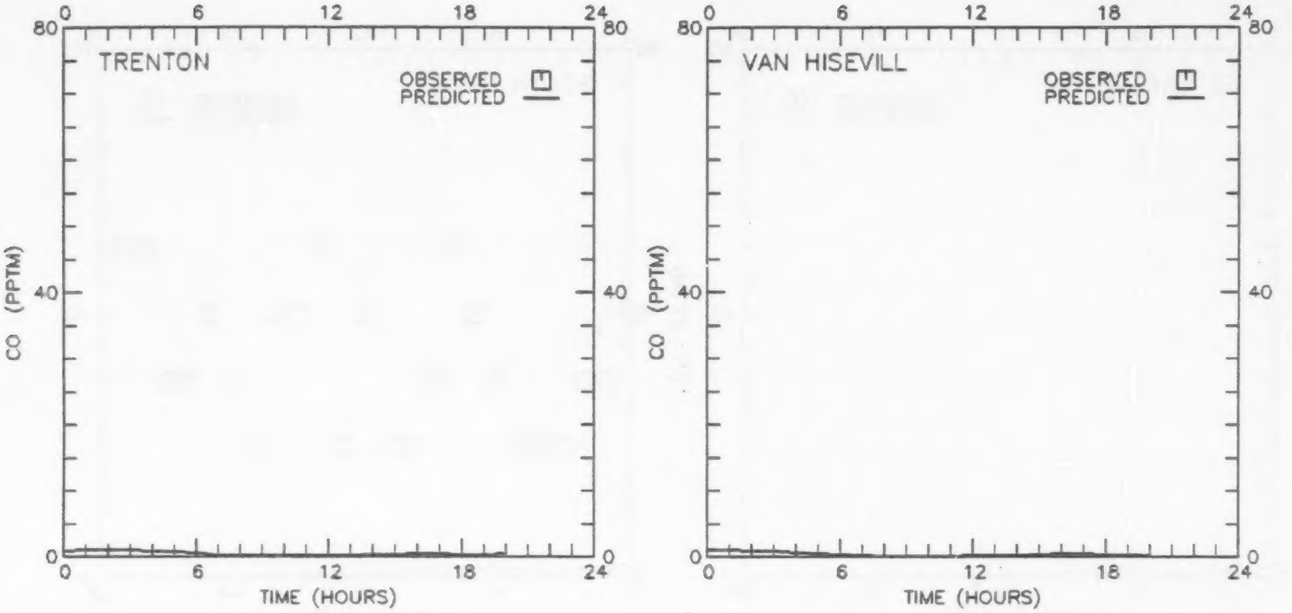
PHILADELPHIA – 7/13/79 – CO – PLANR RUN #1

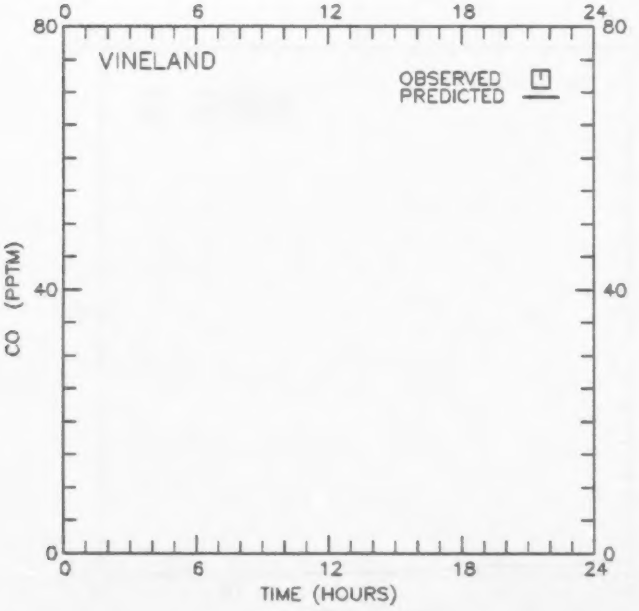


PHILADELPHIA – 7/13/79 – CO – PLANR RUN #1



PHILADELPHIA – 7/13/79 – CO – PLANR RUN #1

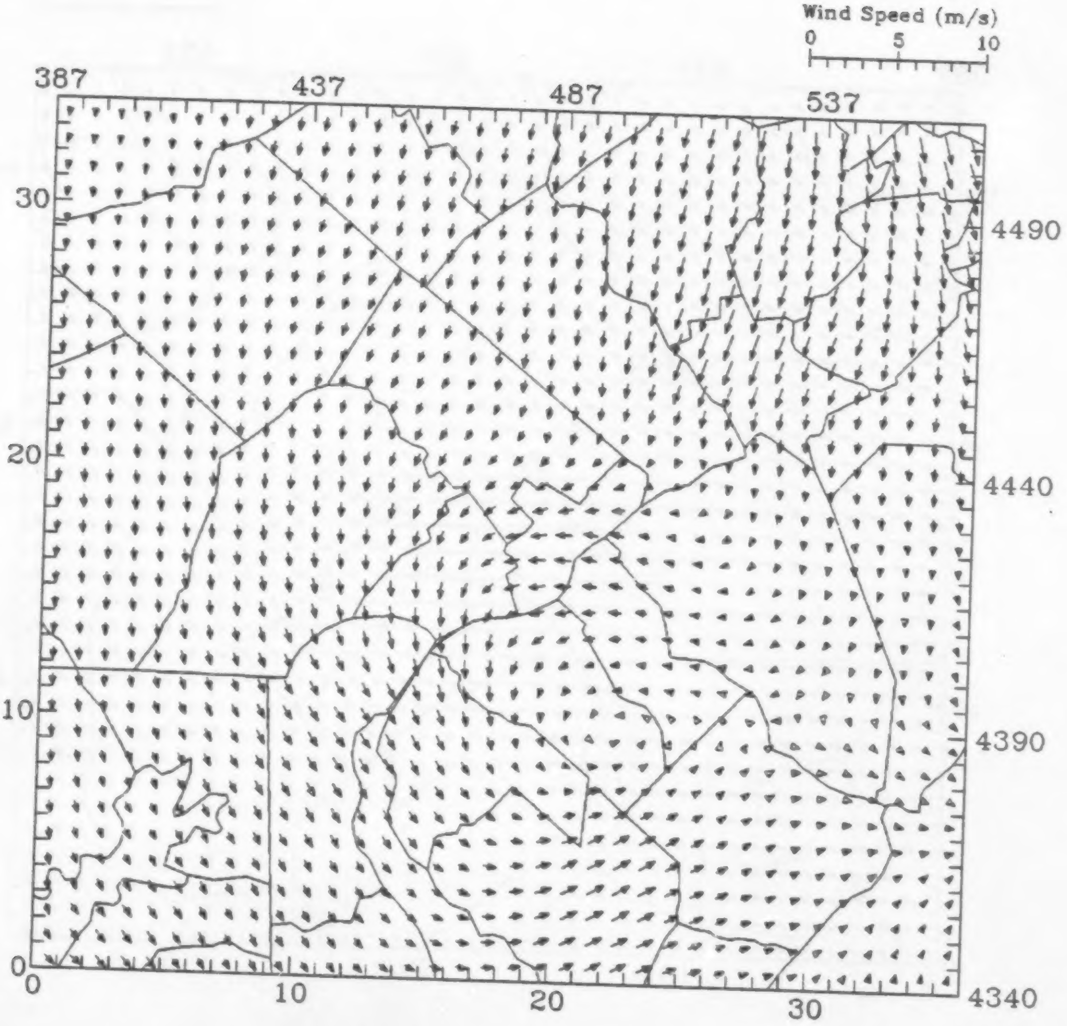




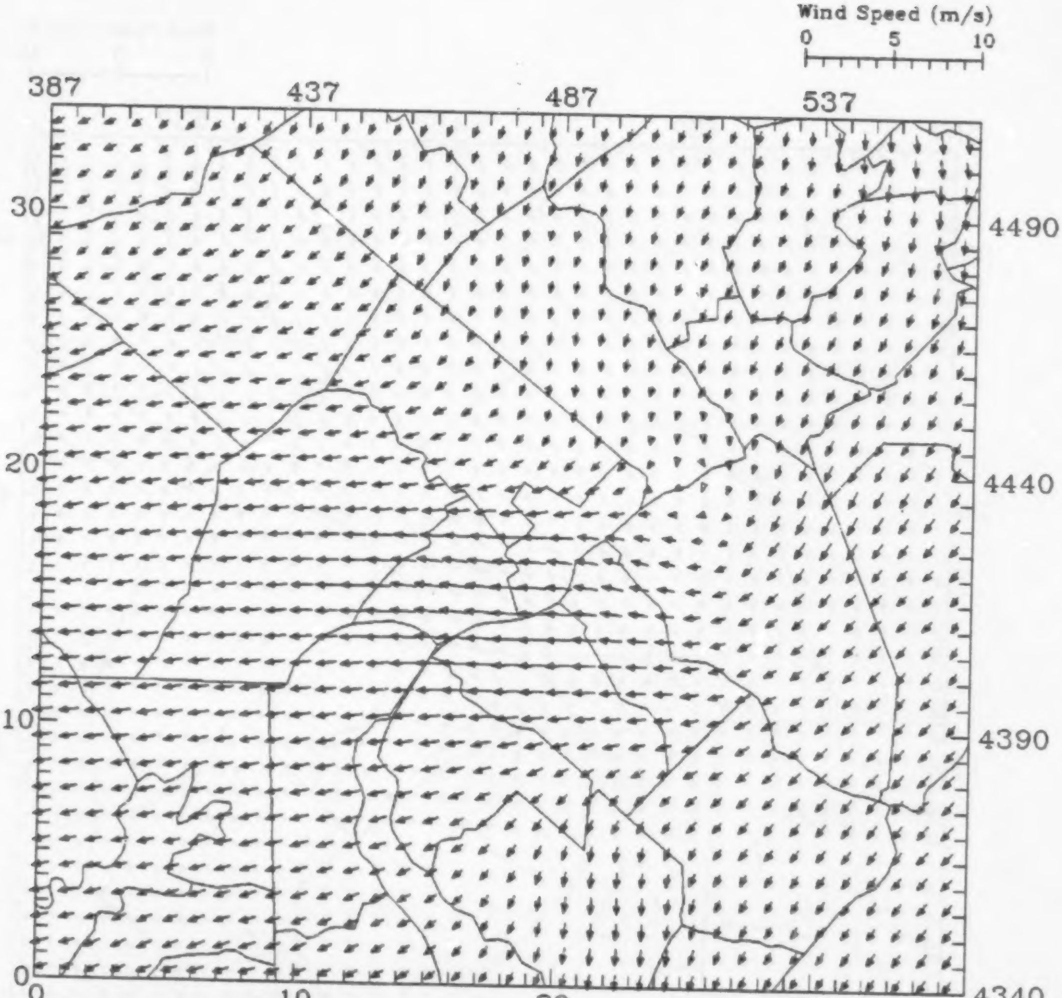
PHILADELPHIA – 7/13/79 – CO – PLANR RUN #1

Appendix E

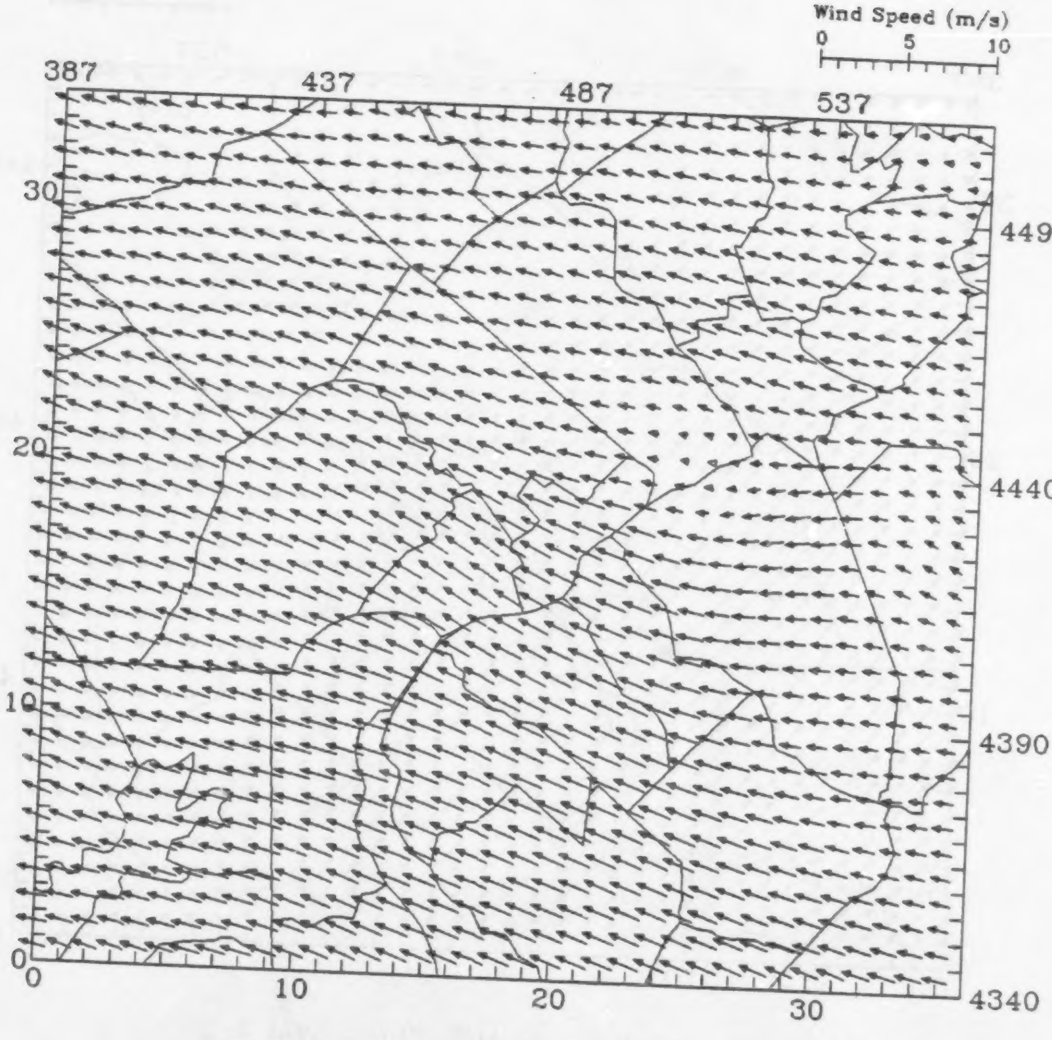
WIND FIELDS USED IN DIAGNOSTIC RUN 2 APPLICATION TO PHILADELPHIA


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

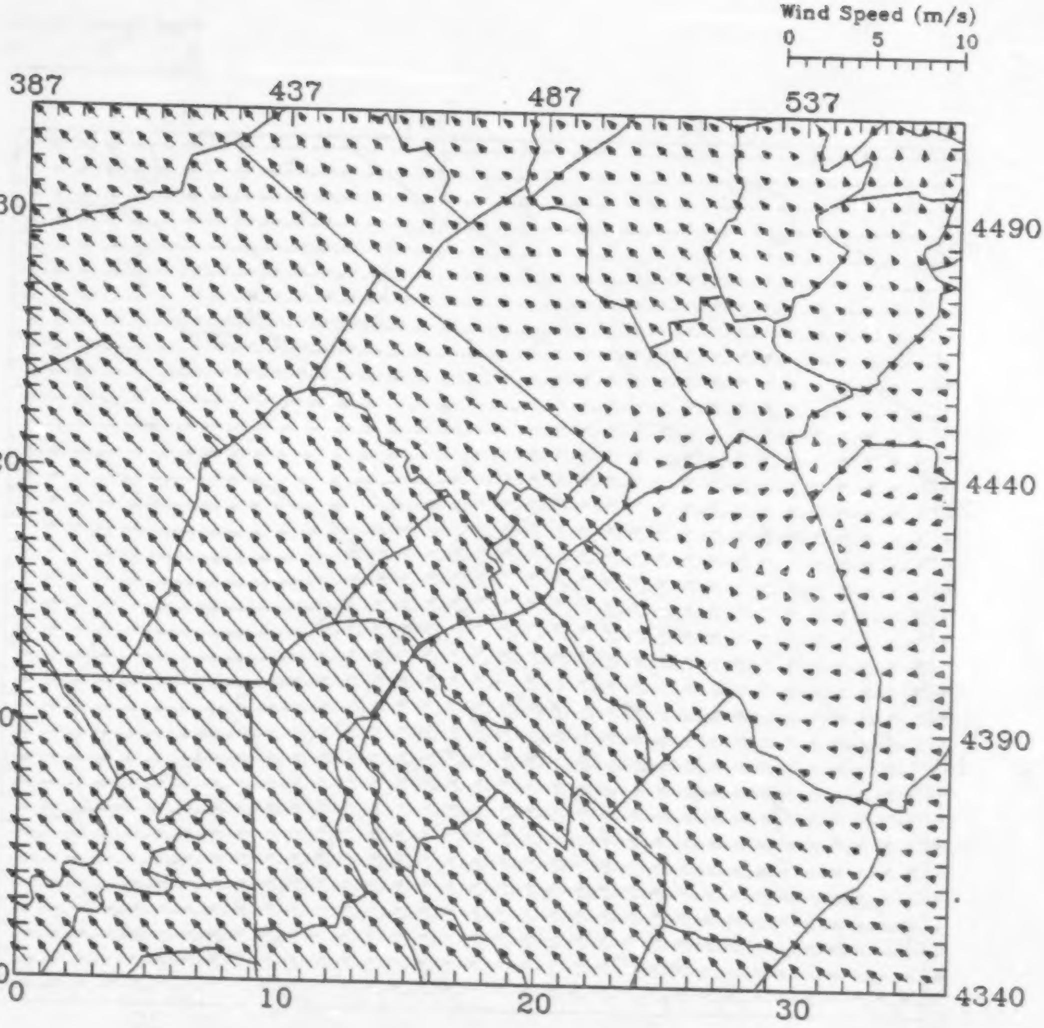
Philadelphia PLANR Winds Eval # 2
Layer 1 at hour 7 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

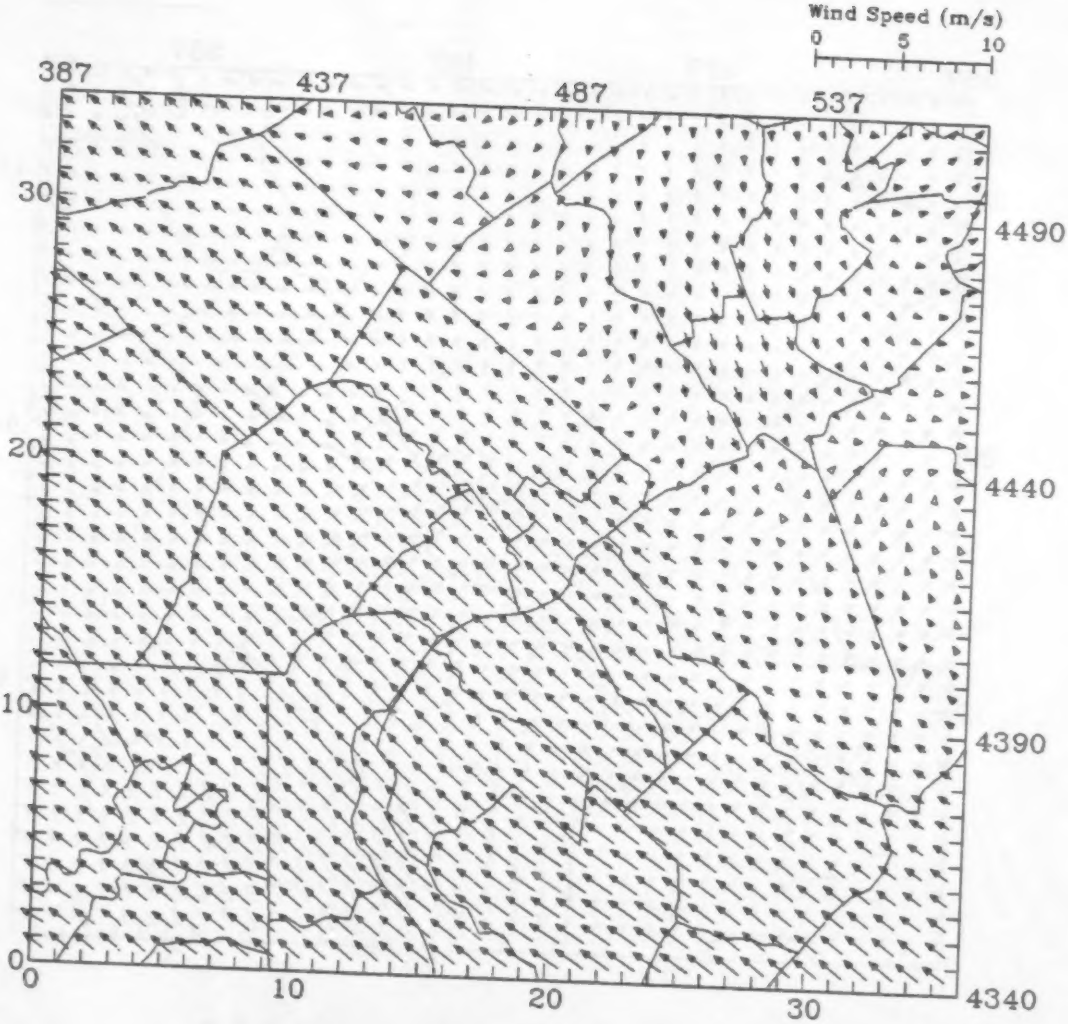
Philadelphia PLANR Winds Eval # 2
Layer 1 at hour 8 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
4490
4440
4390
4340
0
10
20
30

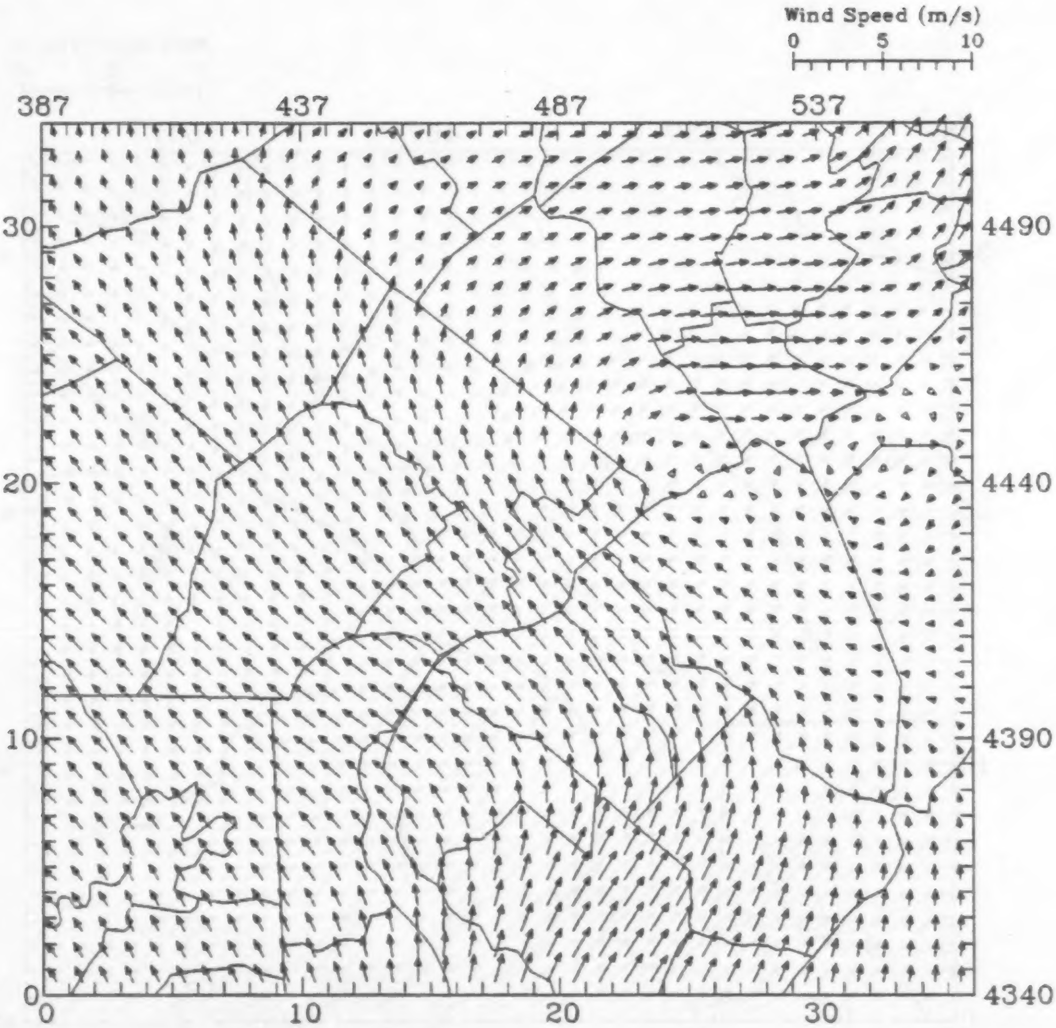
Philadelphia PLANR Winds Eval # 2
Layer 1 at hour 9 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

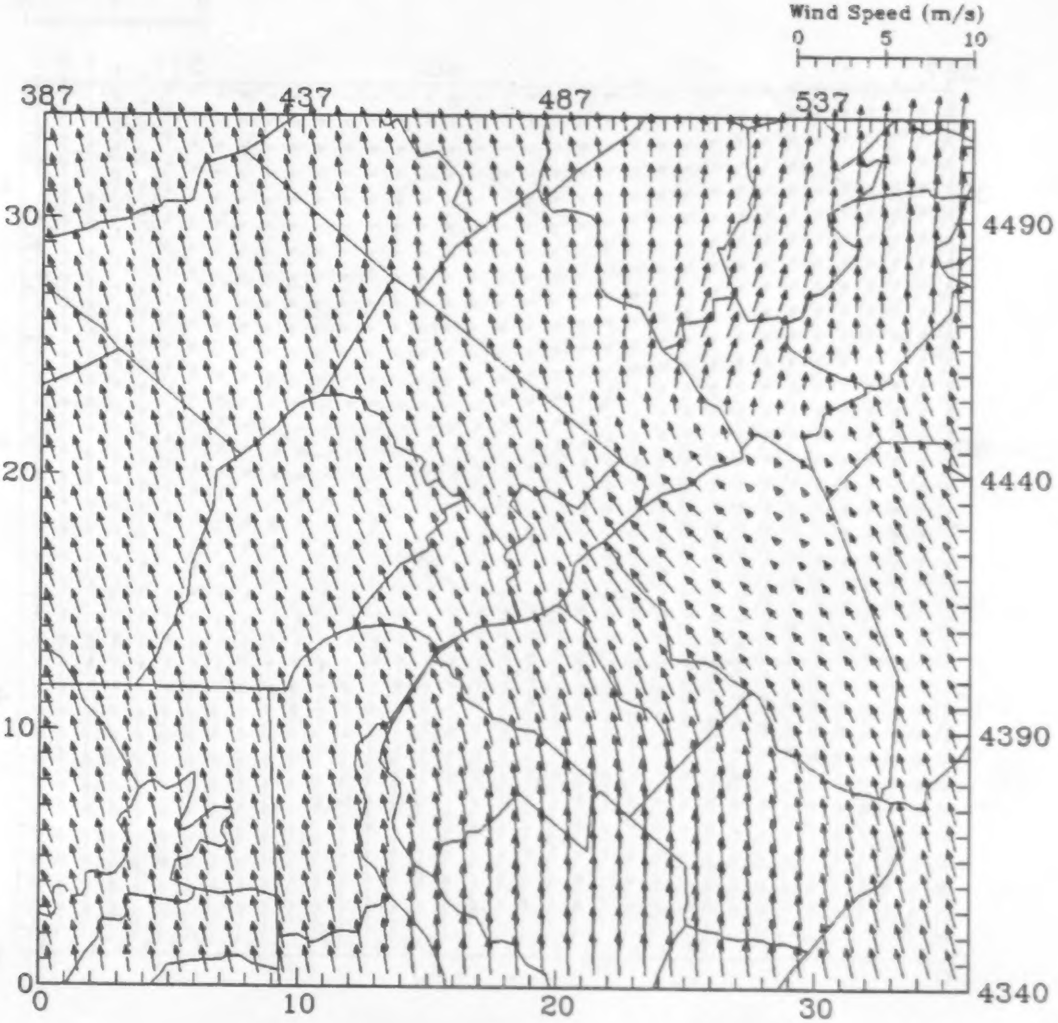
Philadelphia PLANR Winds Eval # 2
Layer 1 at hour 10 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
4490
4440
4390
4340
30
20
10
0
0
10
20
30

Philadelphia PLANR Winds Eval # 2
Layer 1 at hour 11 on 84194

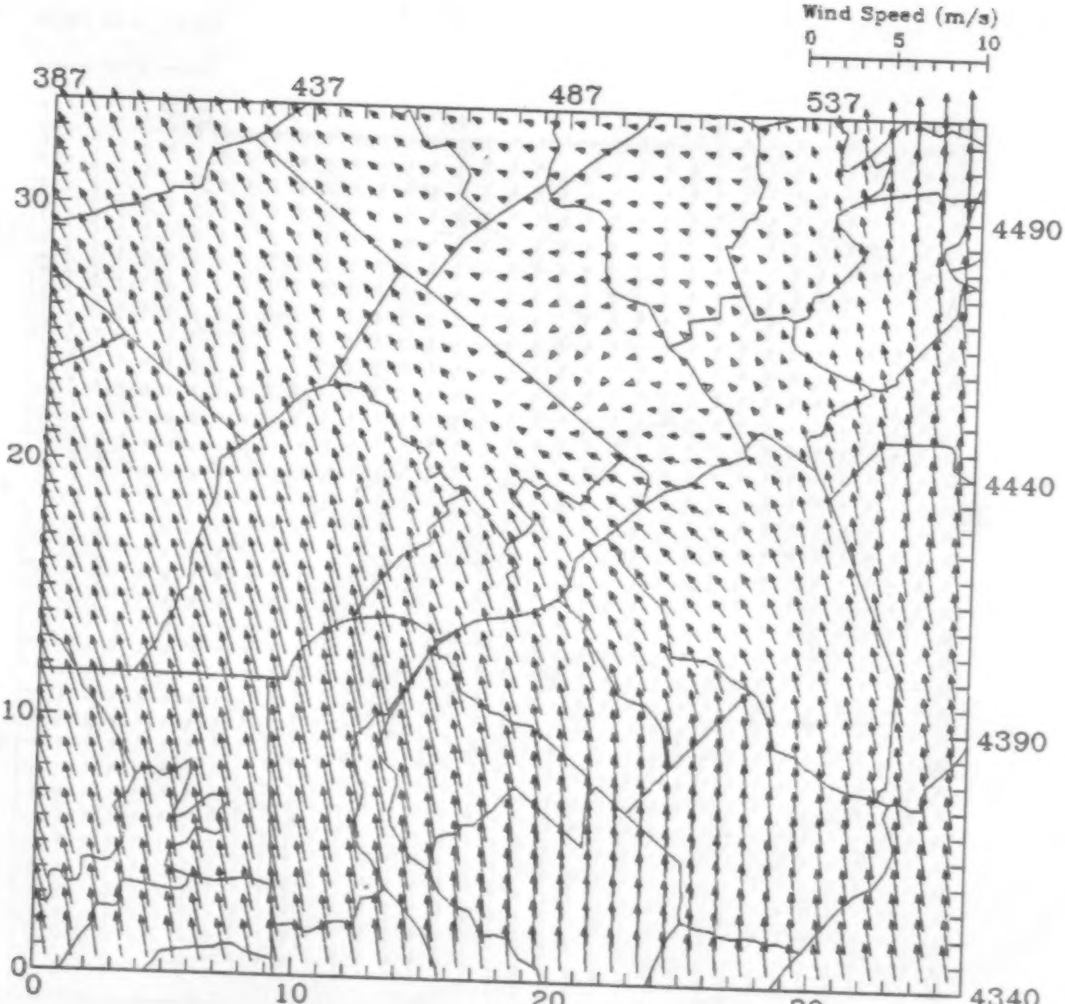

Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

Philadelphia PLANR Winds Eval # 2
Layer 1 at hour 12 on 84194

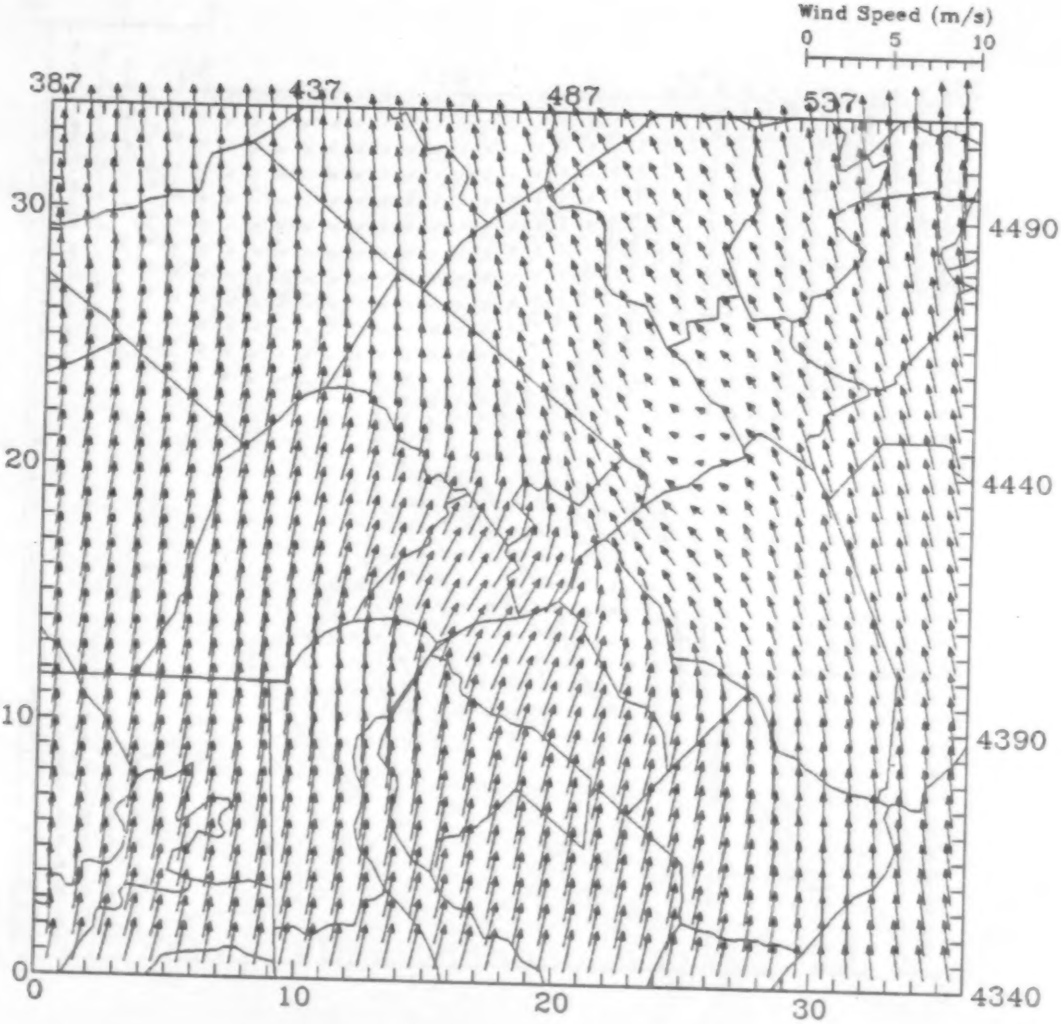


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

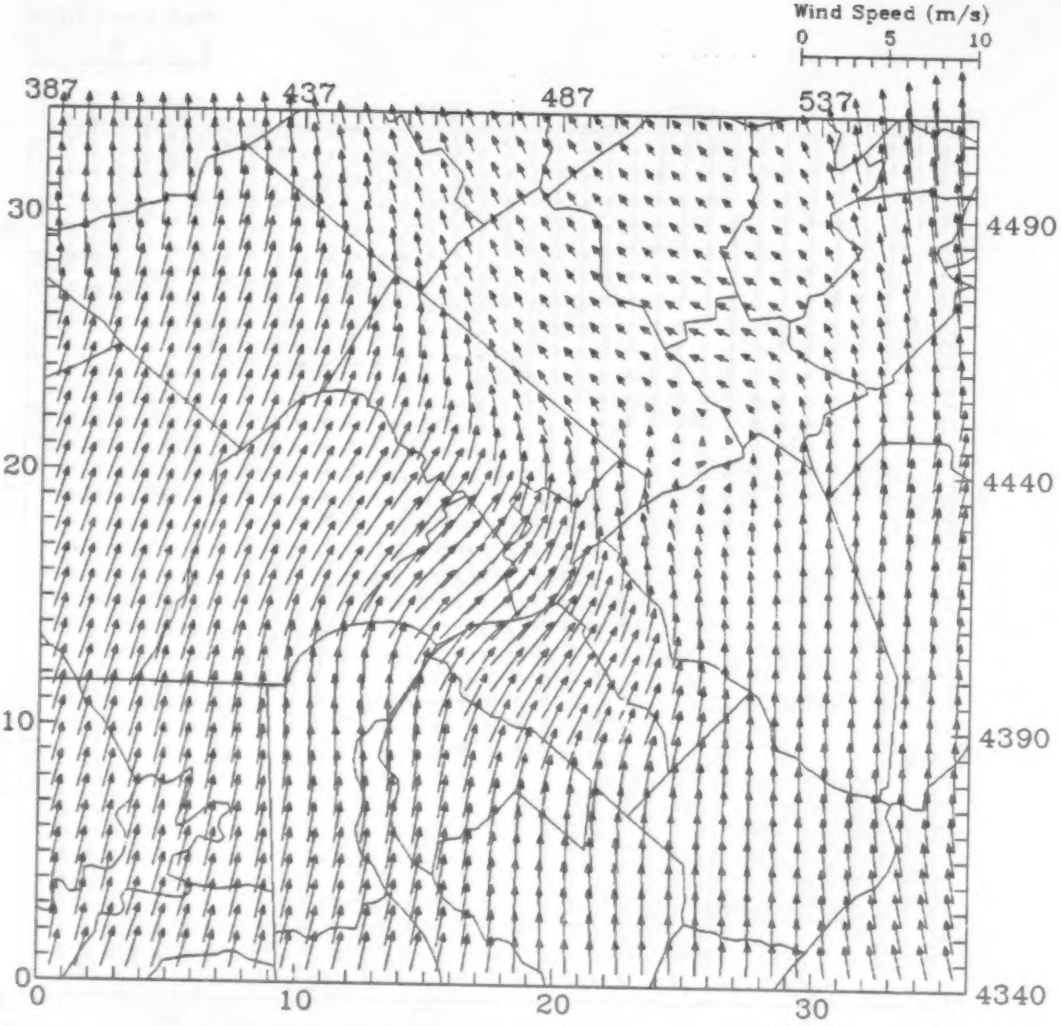
Philadelphia PLANR Winds Eval # 2
Layer 1 at hour 13 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

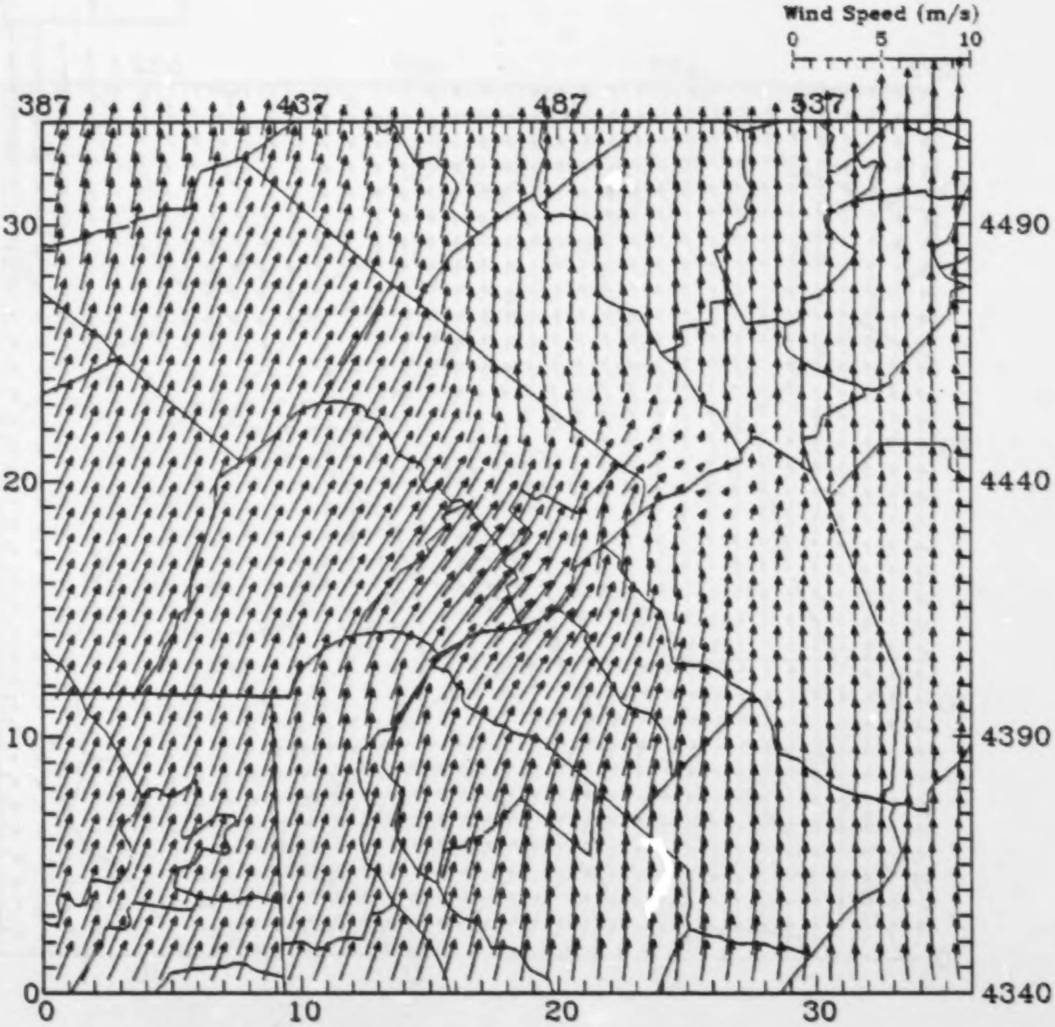
Philadelphia PLANR Winds Eval # 2
Layer 1 at hour 14 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

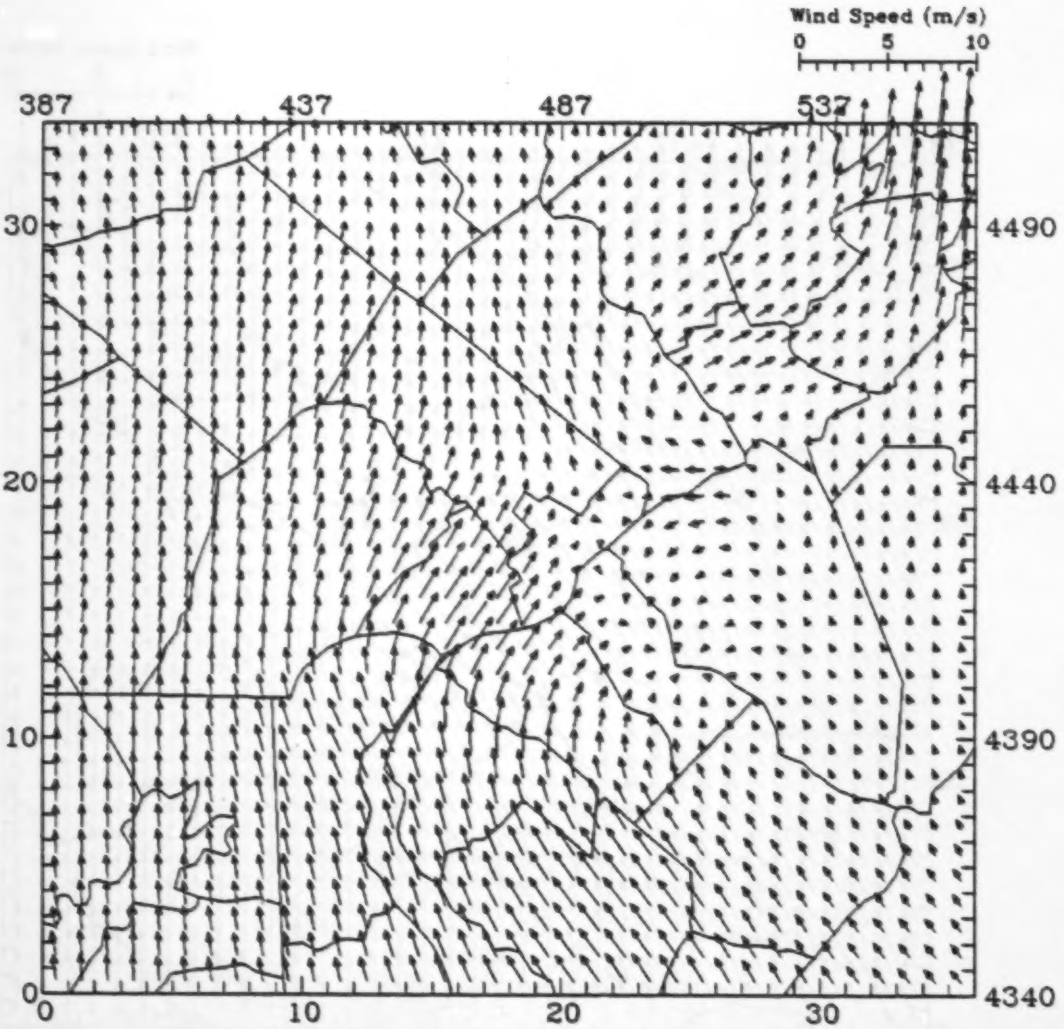
Philadelphia PLANR Winds Eval # 2
Layer 1 at hour 15 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

Philadelphia PLANR Winds Eval # 2
Layer 1 at hour 16 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
0
10
20
30
4490
4440
4390
4340

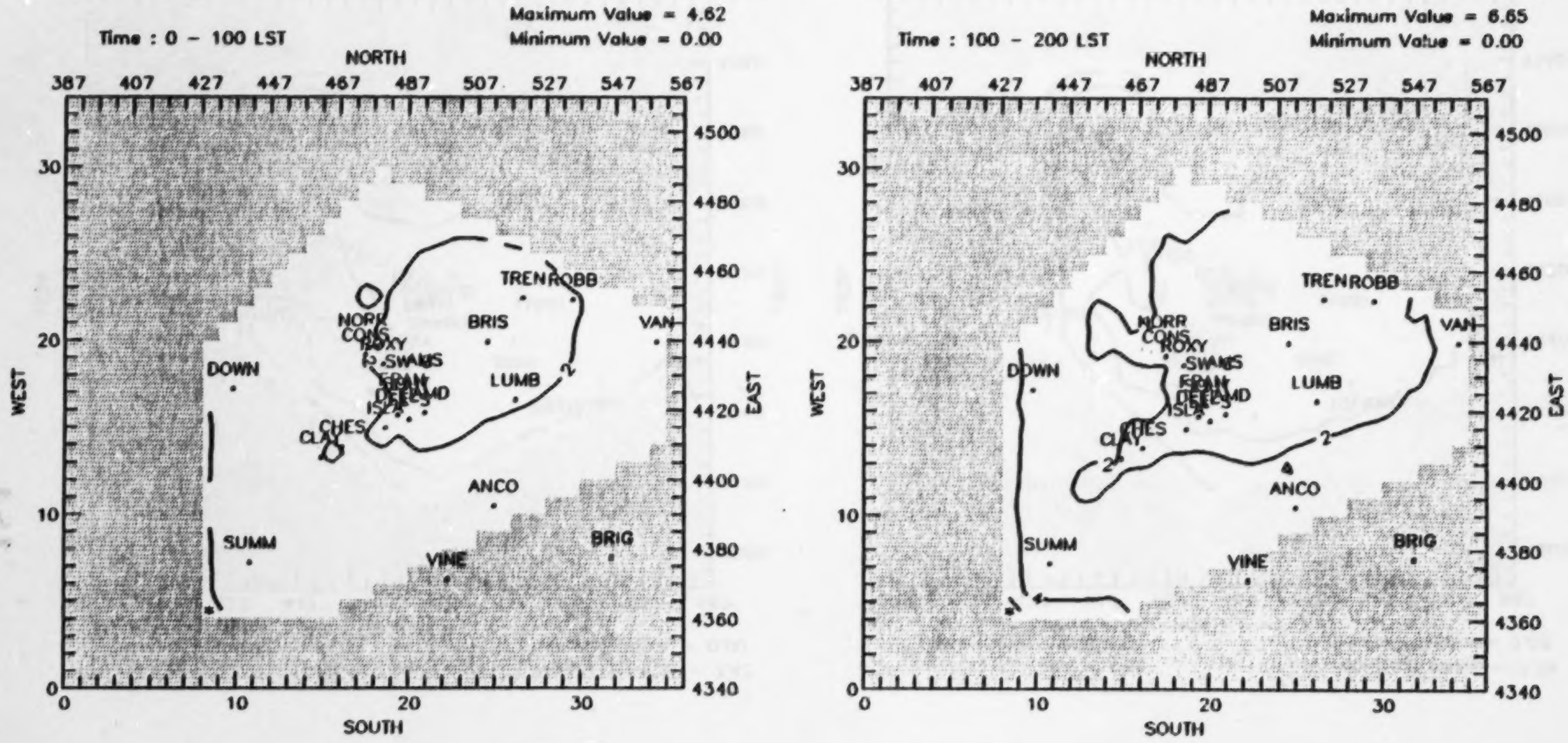
Philadelphia PLANR Winds Eval # 2
Layer 1 at hour 17 on 84194


Wind Speed (m/s)
0
5
10
387
437
487
537
30
20
10
0
4490
4440
4390
4340
0
10
20
30

Philadelphia PLANR Winds Eval # 2
Layer 1 at hour 18 on 84194

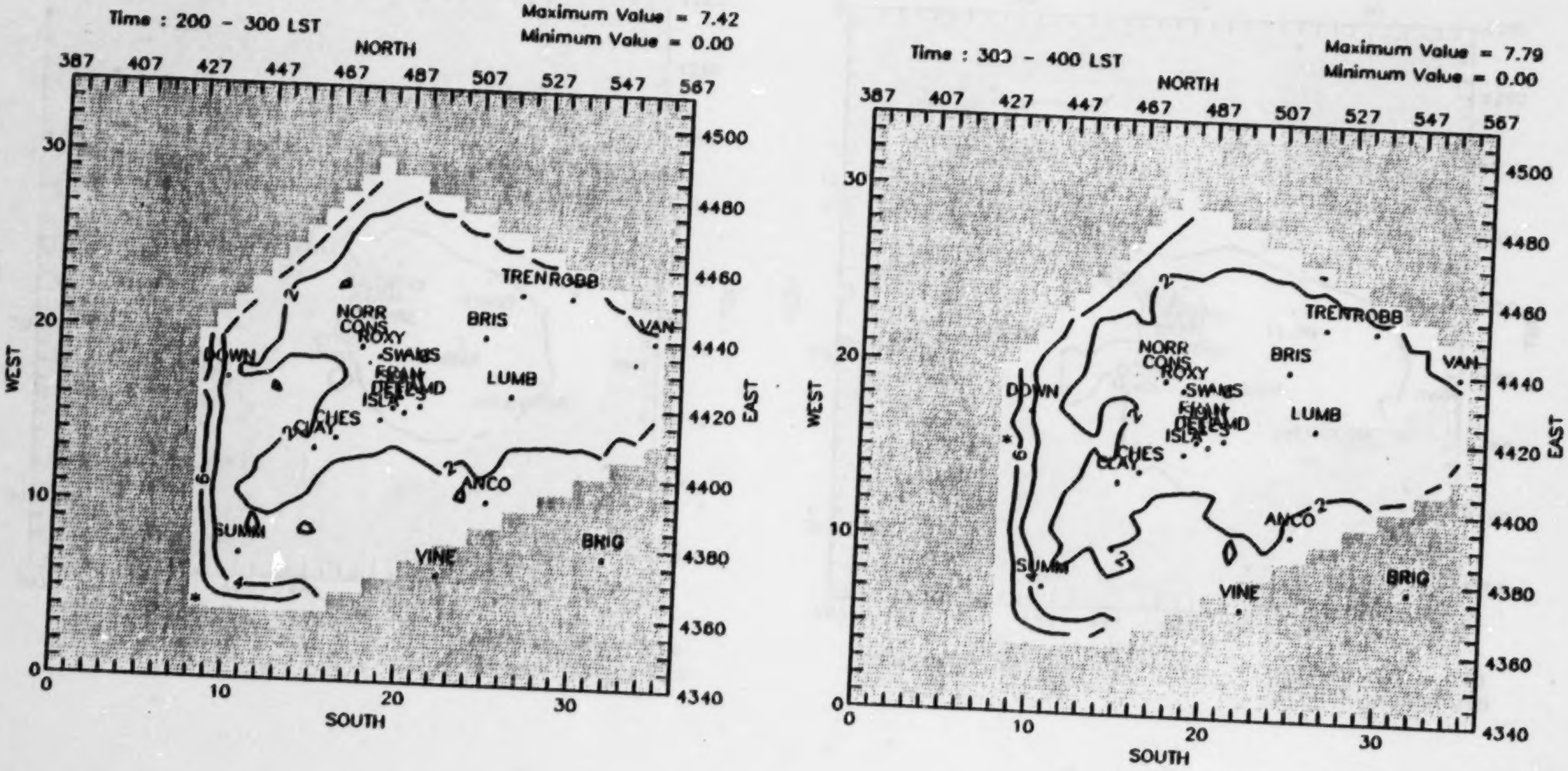
Appendix F

HOURLY OZONE CONCENTRATIONS IN PHILADELPHIA PREDICTED FROM DIAGNOSTIC RUN 2

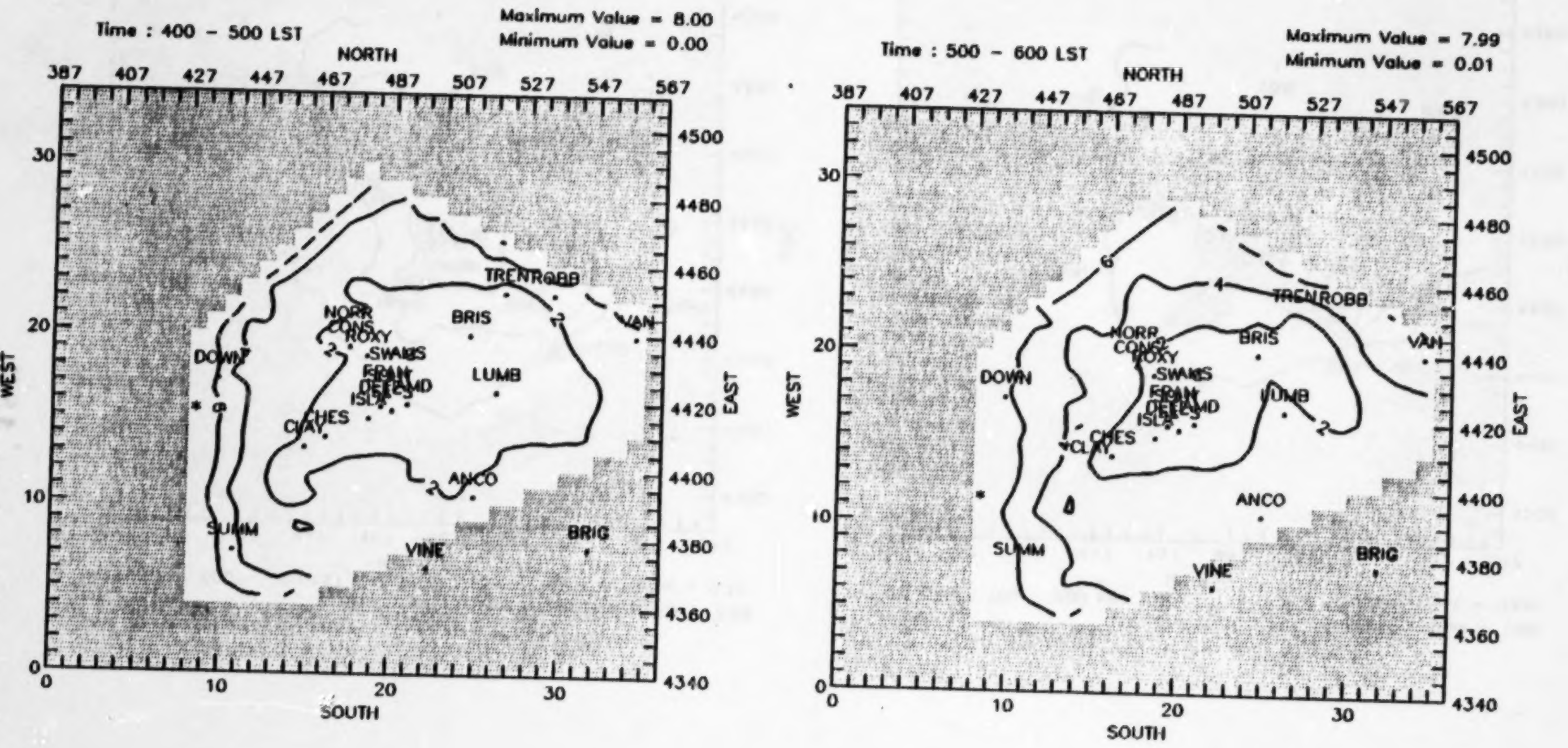


Time : 0 - 100 LST
Maximum Value = 4.62
Minimum Value = 0.00
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
BRIS
VAN
NORR
CONS
ROXY
SWANS
FRAN
DELCES
AMD
ISL
LUMB
DOWN
CHES
CLAY
ANCO
SUMM
VINE
BRIG
2
Time : 100 - 200 LST
Maximum Value = 6.65
Minimum Value = 0.00

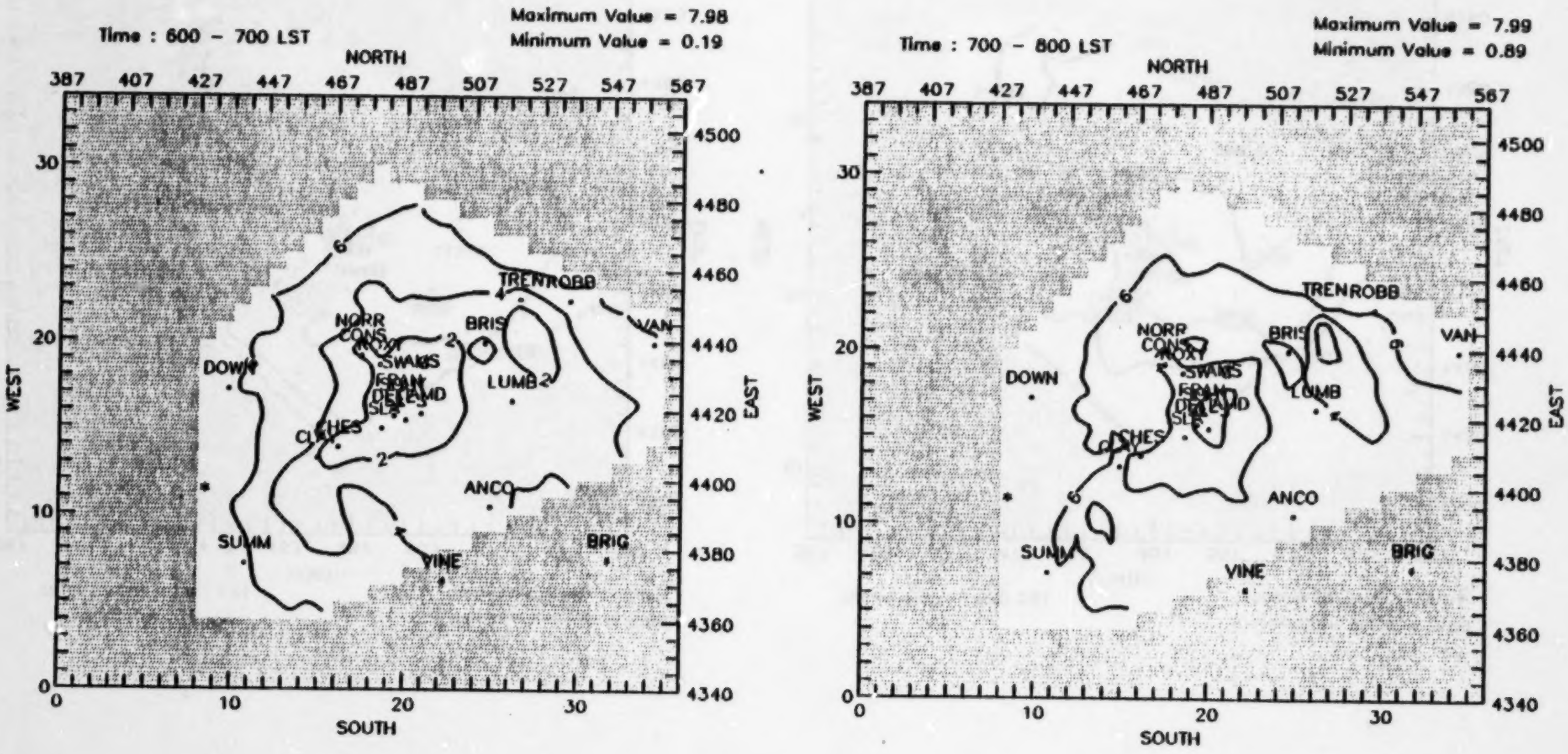
Ozone (pphm) 1979 base emissions, July 13, 1979 (planr2)


Time : 200 - 300 LST
Maximum Value = 7.42
Minimum Value = 0.00
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
VAN
NORR
CONS
ROXY
SWANS
FRAN
DETE
AMD
ISLA
BRIS
LUMB
DOWN
CHES
CLAY
ANCO
SUMM
VINE
BRIG
Time : 300 - 400 LST
Maximum Value = 7.79
Minimum Value = 0.00

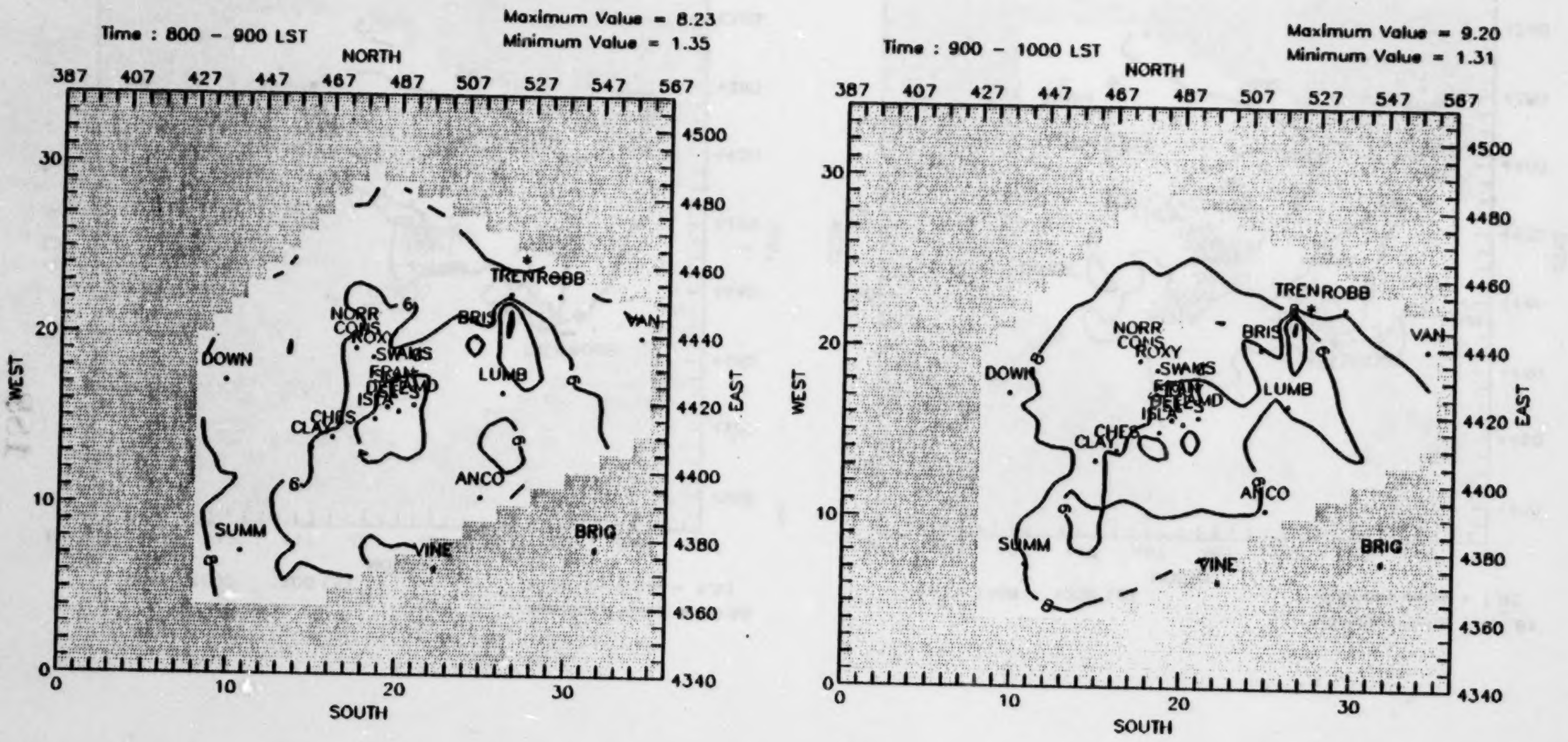
Ozone (pphm) 1979 base emissions, July 13, 1979 (planr2)


Time : 400 - 500 LST
Maximum Value = 8.00
Minimum Value = 0.00
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
0
10
20
30
4340
4360
4380
4400
4420
4440
4460
4480
4500
TRENROBB
VAN
NORR
CONS
ROXY
BRIS
SWANS
FRAN
DEEC
MD
ISLS
LUMB
DOWN
CHES
CLAY
ANCO
SUMM
VINE
BRIG
2
8
Time : 500 - 600 LST
Maximum Value = 7.99
Minimum Value = 0.01
6
4
2

Ozone (pphm) 1979 base emissions, July 13, 1979 (planr2)

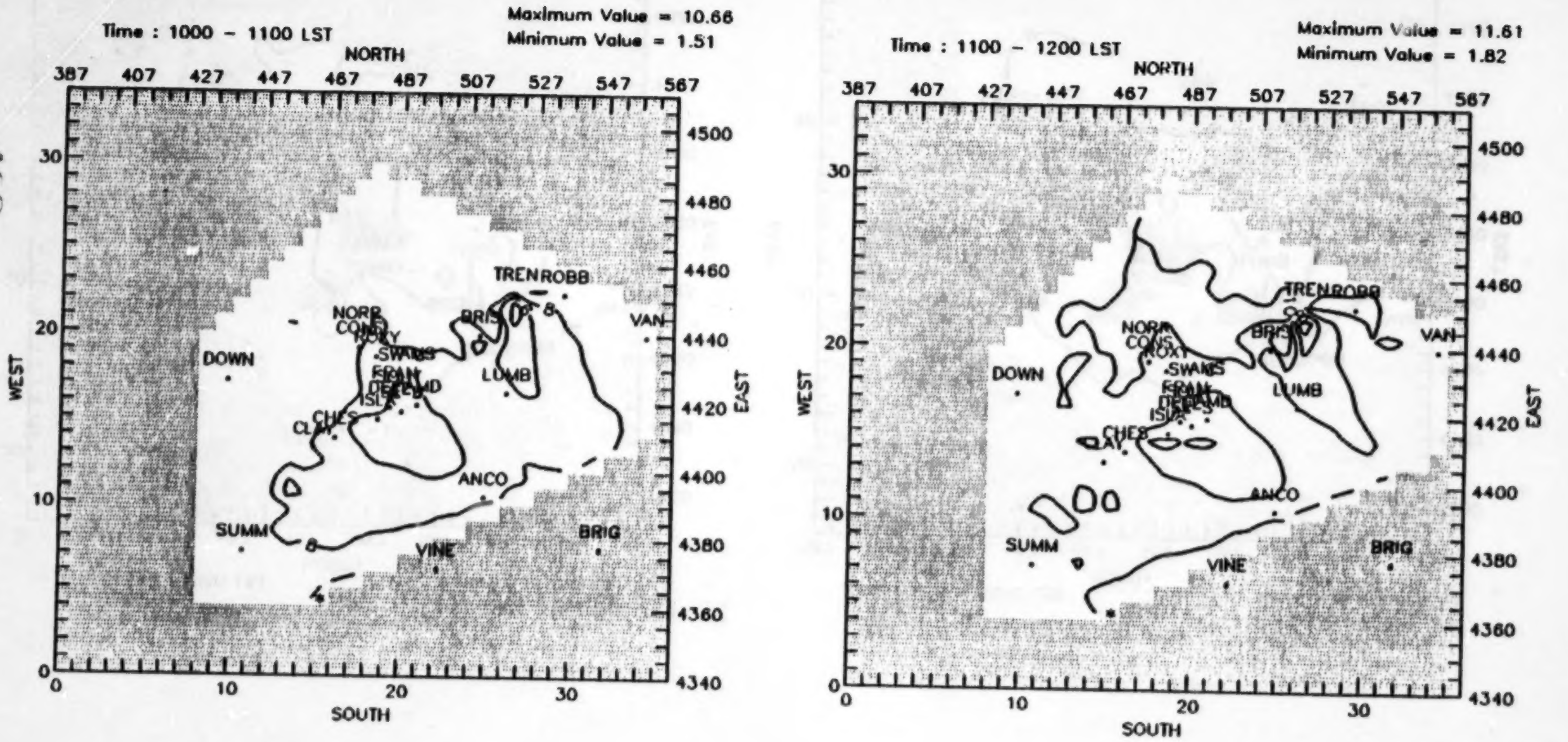

Time : 600 - 700 LST
Maximum Value = 7.98
Minimum Value = 0.19
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
VAN
NORR
CONS
ROXY
SWAKS
FRAN
DETAMD
SLS
BRIS
LUMB
DOWN
CHES
CLAR
ANCO
SUMM
VINE
BRIG
2
4
6
Time : 700 - 800 LST
Maximum Value = 7.99
Minimum Value = 0.89

Ozone (pphm) 1979 base emissions, July 13, 1979 (planr2)

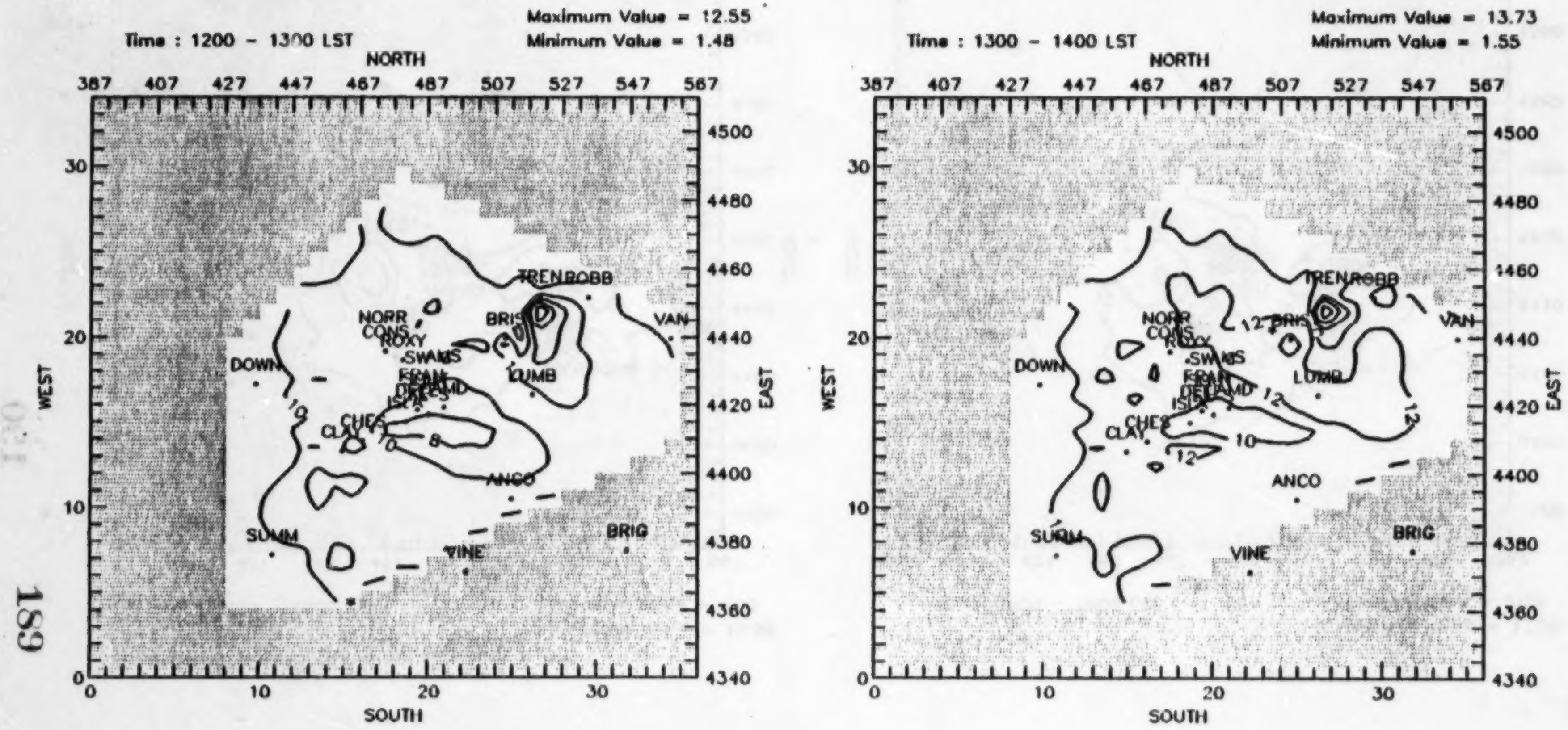


Time : 800 - 900 LST
Maximum Value = 8.23
Minimum Value = 1.35
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
NORR
CONS
ROXY
SWANS
FRAN
DEEL
AMD
ISLA
CHES
CLAY
DOWN
BRIS
LUMB
VAN
ANCO
SUMM
VINE
BRIG
6
Time : 900 - 1000 LST
Maximum Value = 9.20
Minimum Value = 1.31

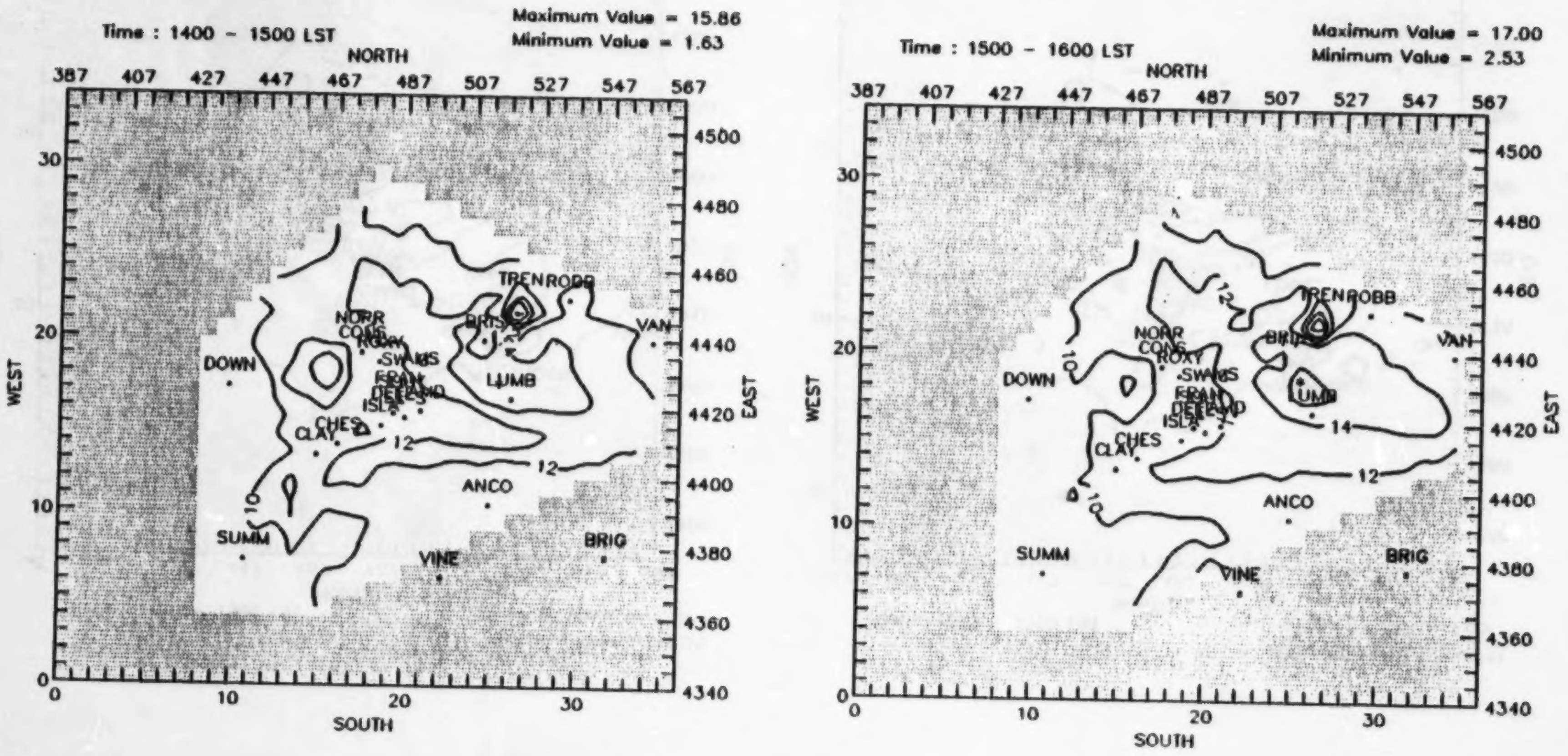
Ozone (pphm) 1979 base emissions, July 13, 1979 (planr2)


Time : 1000 - 1100 LST
Maximum Value = 10.66
Minimum Value = 1.51
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
NORR
CONS
ROXY
SWANS
FRAN
DEFE
LMD
ISLA
CHES
CLAY
BRIS
LUMB
VAN
DOWN
ANCO
SUMM
VINE
BRIG
8
4
Time : 1100 - 1200 LST
Maximum Value = 11.61
Minimum Value = 1.82

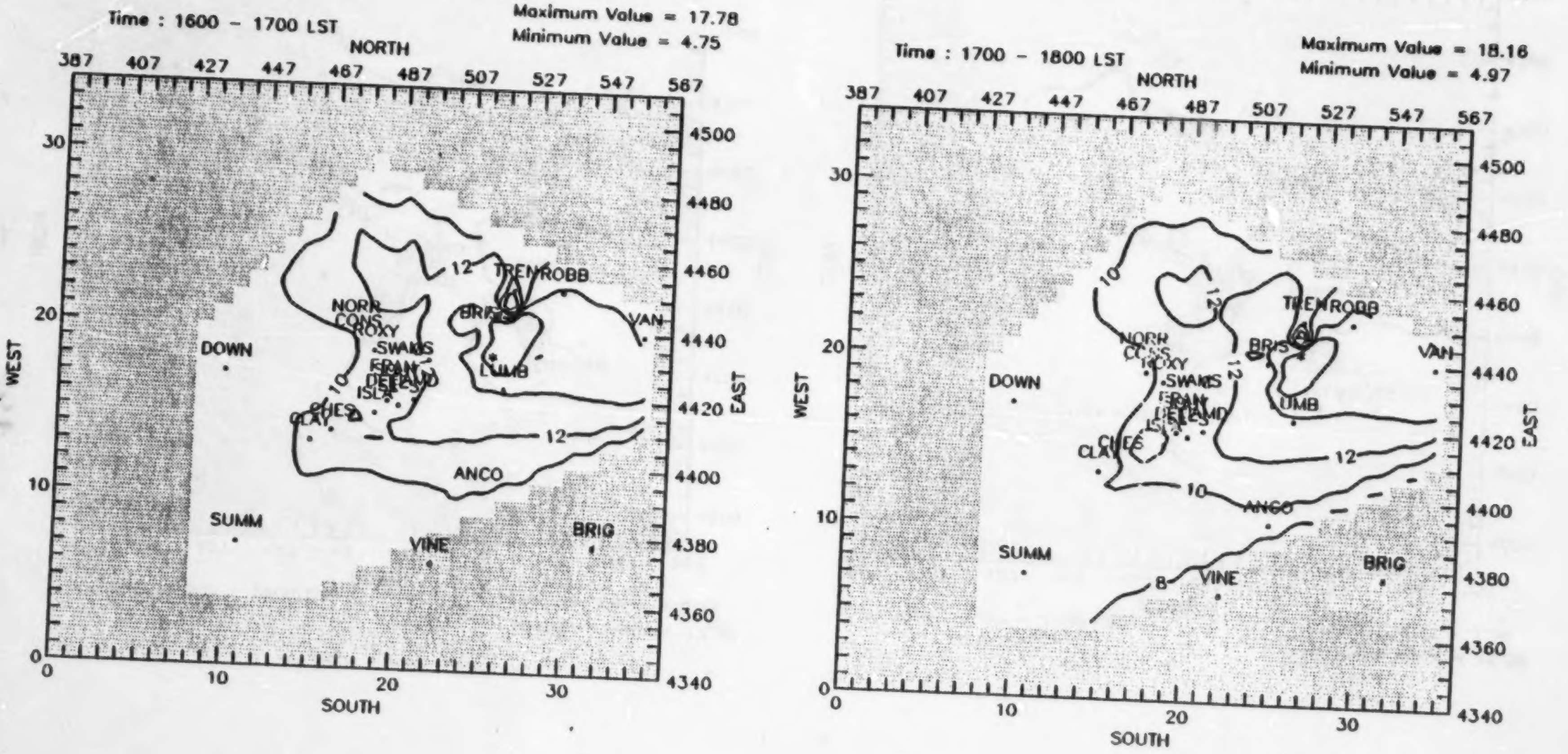
Ozone (pphm) 1979 base emissions, July 13, 1979 (planr2)


Time : 1200 - 1300 LST
Maximum Value = 12.55
Minimum Value = 1.48
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
NORR
CONS
ROXY
SWANS
FRAN
DELAMD
ISL
BRIS
LUMB
VAN
DOWN
CHES
CLAY
ANCO
SUMM
VINE
BRIG
10
8
Time : 1300 - 1400 LST
Maximum Value = 13.73
Minimum Value = 1.55
12
10

Ozone (pphm) 1979 base emissions, July 13, 1979 (planr2)


Time : 1400 - 1500 LST
Maximum Value = 15.86
Minimum Value = 1.63
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
NORR
CONS
ROXY
SWANS
FRAN
DEFEAND
ISLA
CHES
CLAY
DOWN
BRIS
LUMB
VAN
ANCO
SUMM
VINE
BRIG
10
12
12
Time : 1500 - 1600 LST
Maximum Value = 17.00
Minimum Value = 2.53
14
10
12

Ozone (pphm) 1979 base emissions, July 13, 1979 (planr2)

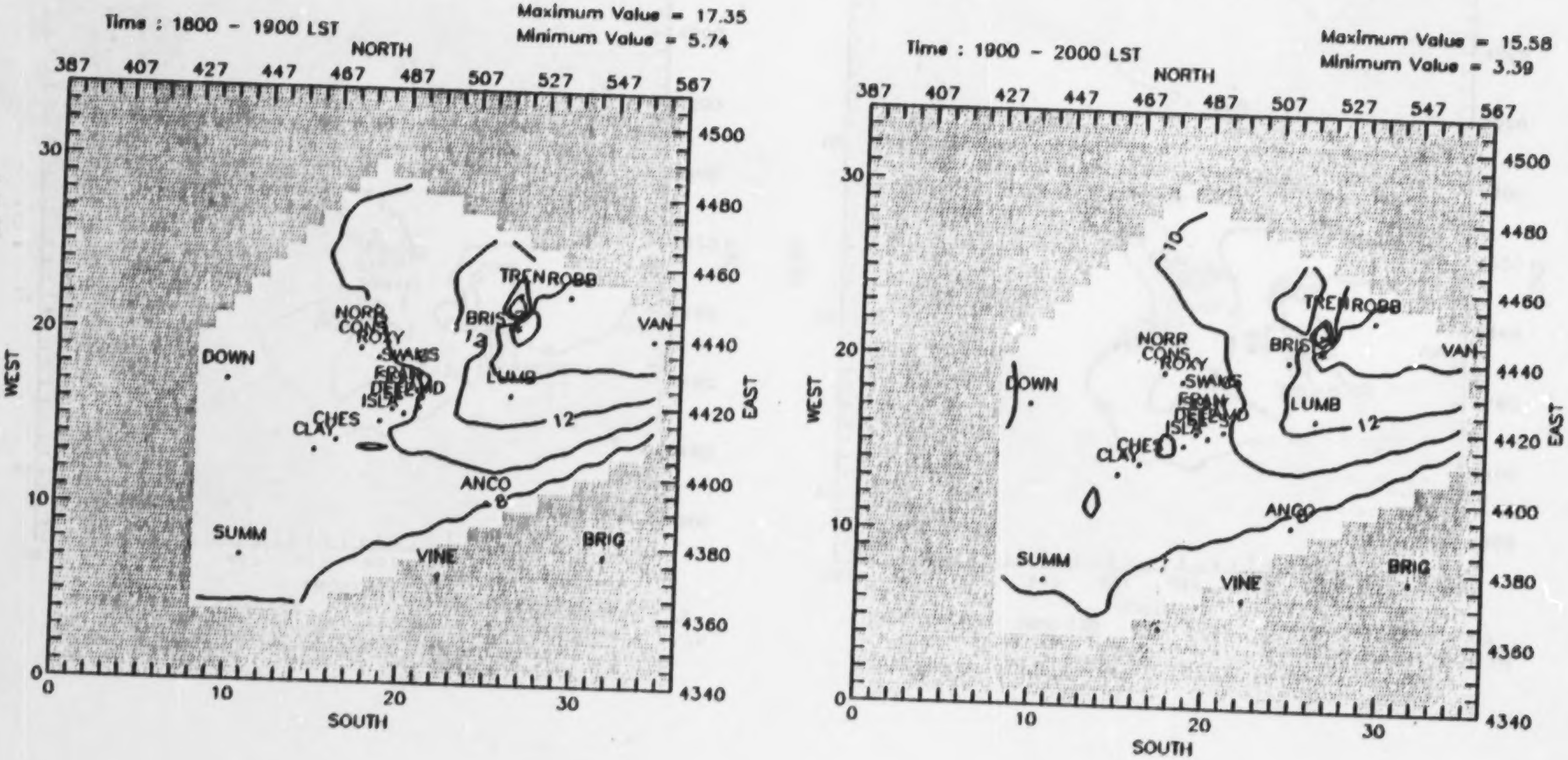


Time : 1600 - 1700 LST Maximum Value = 17.78 Minimum Value = 4.75

Time : 1700 - 1800 LST Maximum Value = 18.16 Minimum Value = 4.97

NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
DOWN
SUMM
VINE
BRIG
ANCO
NORR
CONS
ROXY
SWAKS
FRAN
DEFAND
ISLE
CHES
CLAY
BRIS
TRENROBB
LUMB
VAN
8
10
12

Ozone (pphm) 1979 base emissions, July 13, 1979 (planr2)



Time : 1800 - 1900 LST
Maximum Value = 17.35
Minimum Value = 5.74

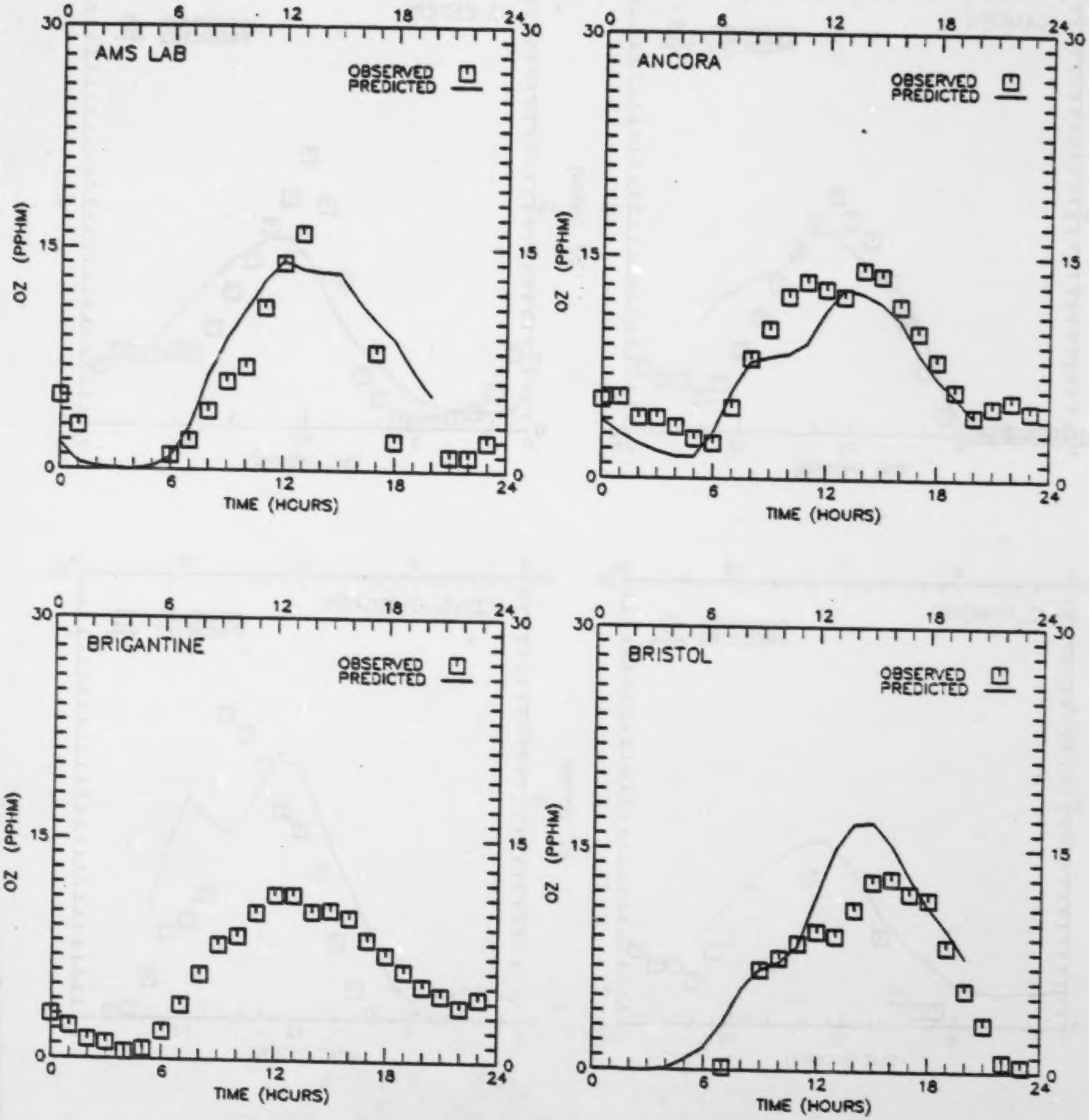
Time : 1900 - 2000 LST
Maximum Value = 15.58
Minimum Value = 3.39

NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
0
10
20
30
4340
4360
4380
4400
4420
4440
4460
4480
4500
DOWN
SUMM
NORR
CONS
ROXY
SWANS
FRAN
DEEP
ISLE
CHES
CLAY
BRIS
TREN
ROBB
LUMB
VAN
ANCO
VINE
BRIG
12
13
8
10

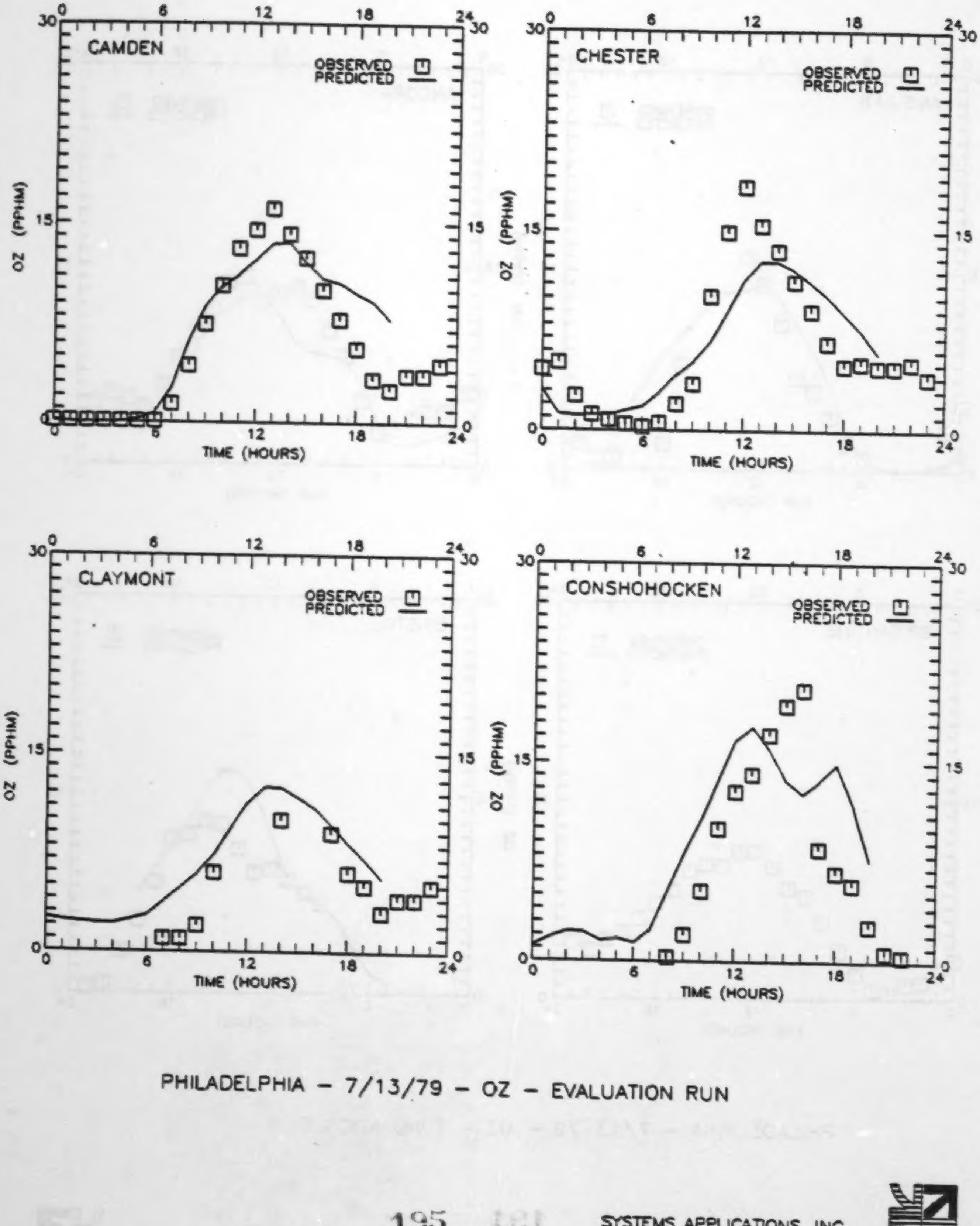
Ozone (pphm) 1979 base emissions, July 13, 1979 (planr2)

Appendix G

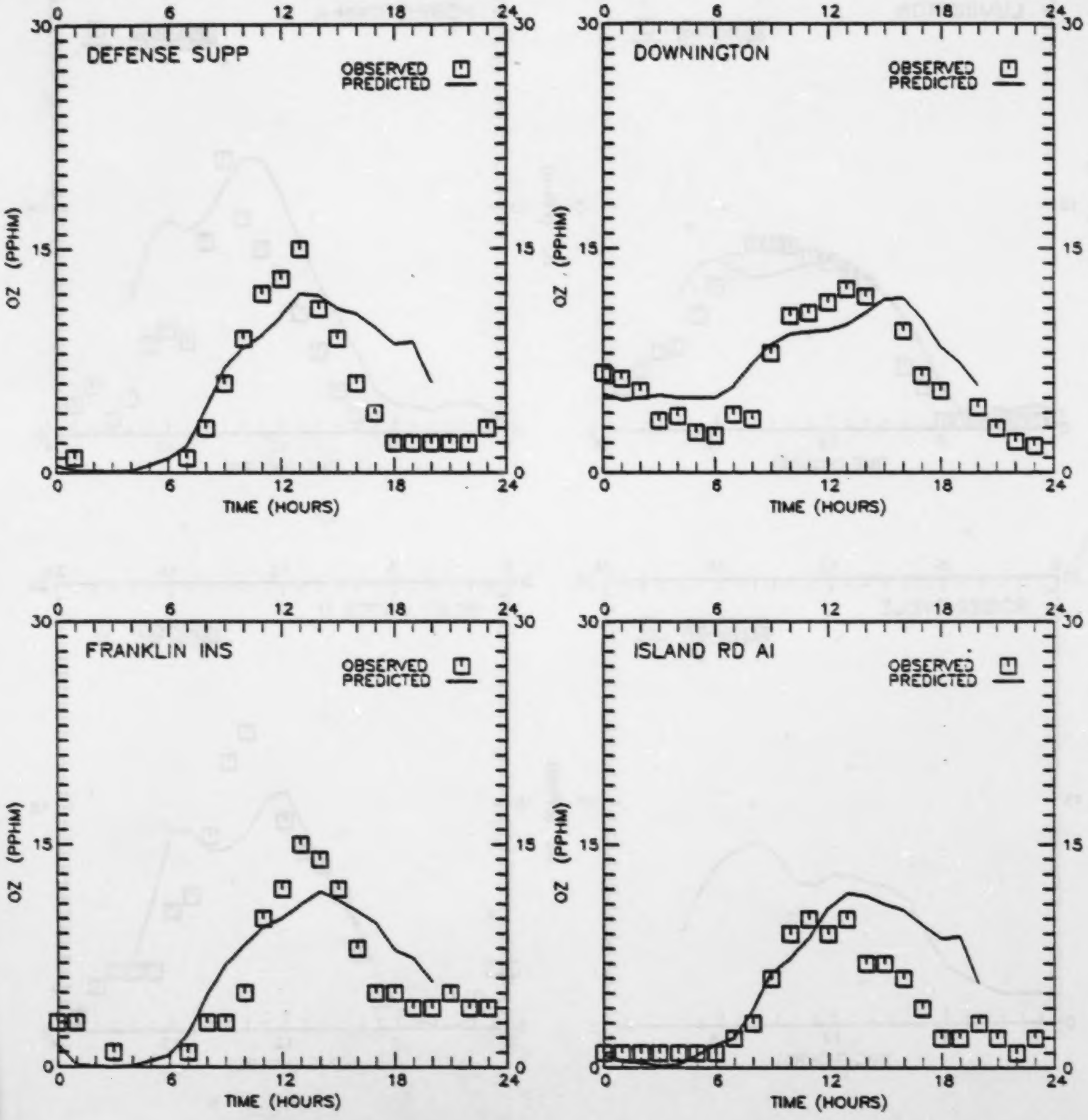
TIME SERIES OF PREDICTED AND OBSERVED HOURLY OZONE, NO, NO_2, AND CO CONCENTRATIONS IN PHILADELPHIA FOR THE UAM(CB-IV) USING A RICH DATA BASE (POS UAM)



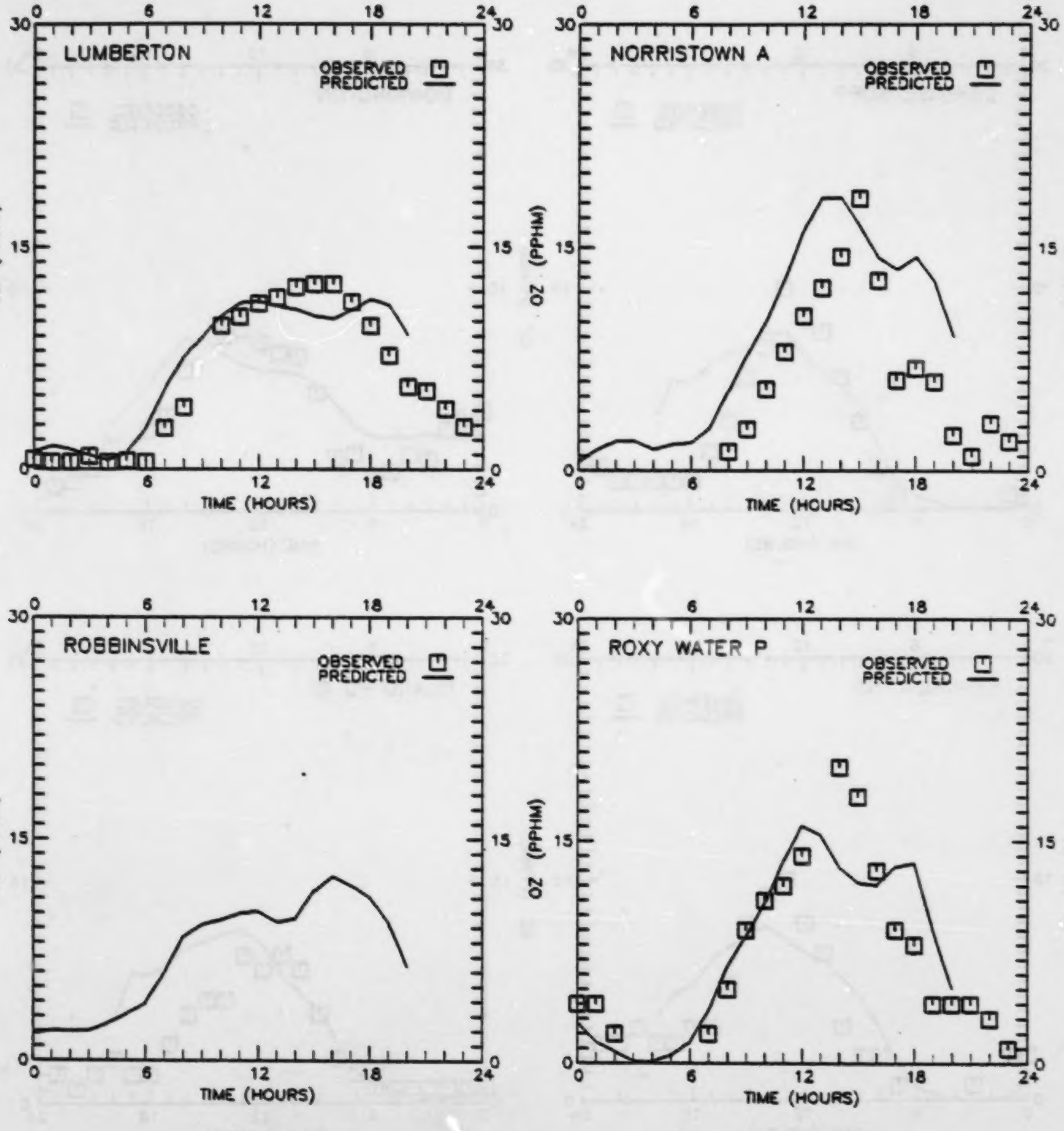
PHILADELPHIA – 7/13/79 – OZ – EVALUATION RUN



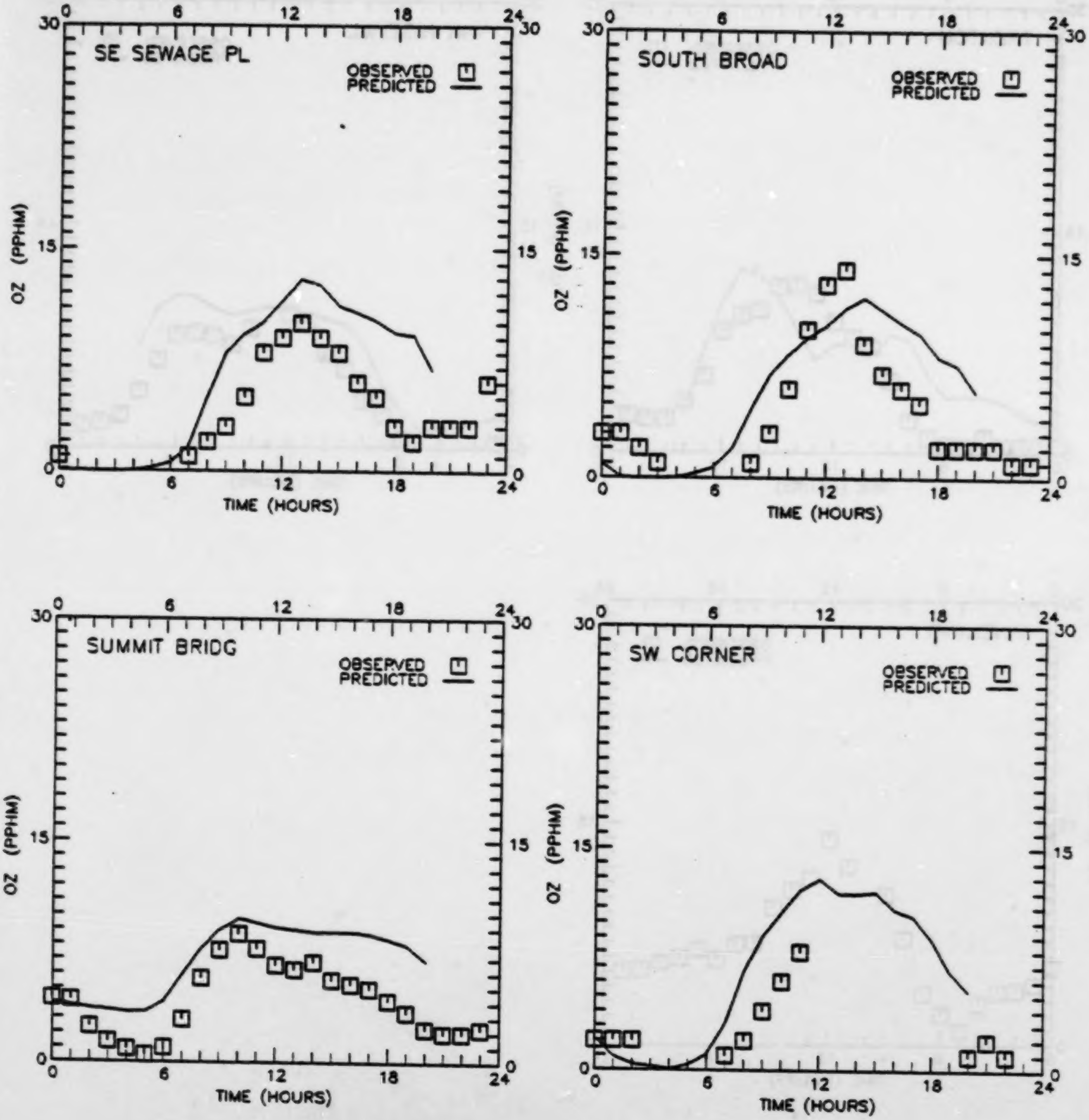
PHILADELPHIA – 7/13/79 – OZ – EVALUATION RUN



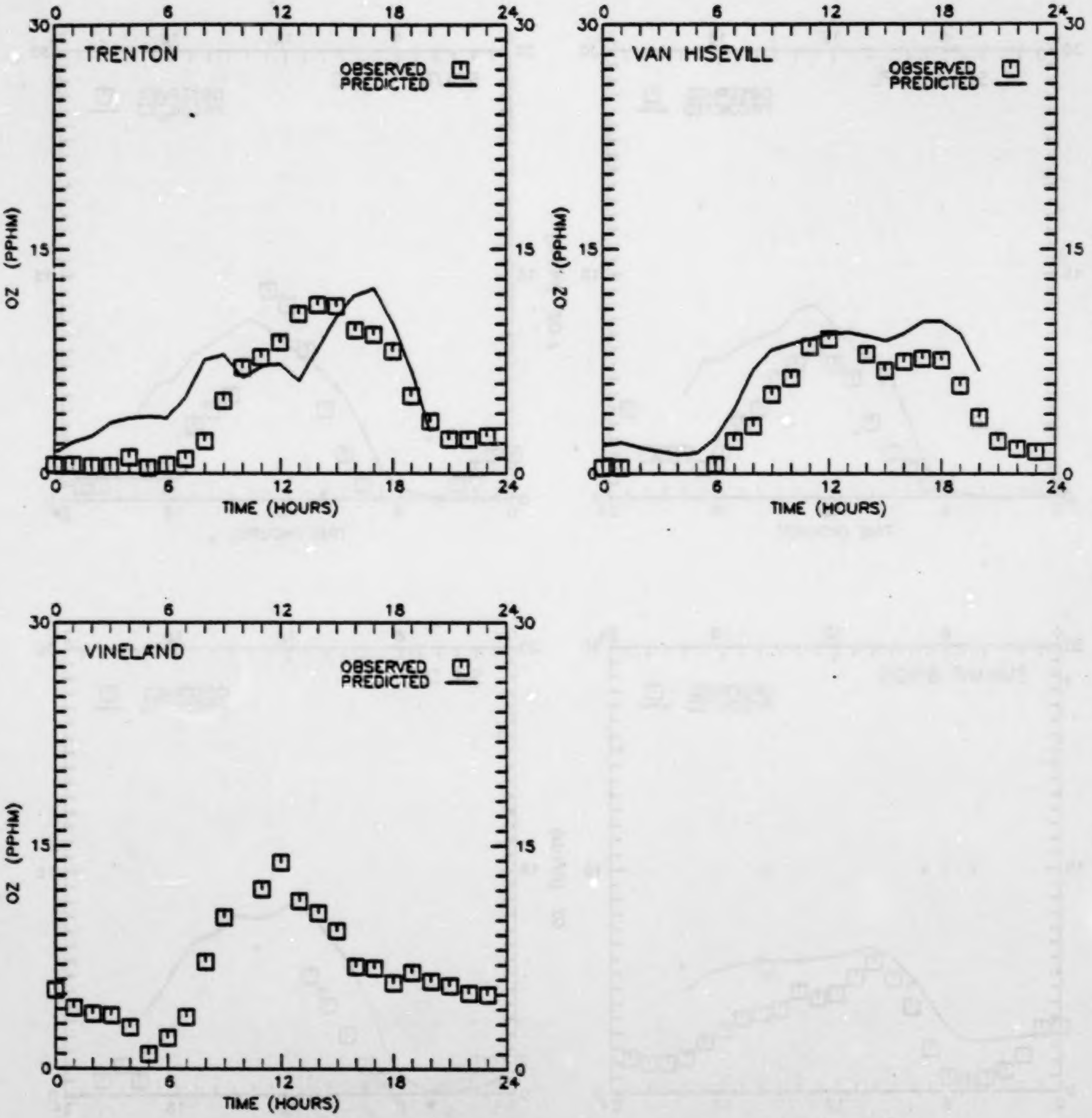
PHILADELPHIA – 7/13/79 – OZ – EVALUATION RUN



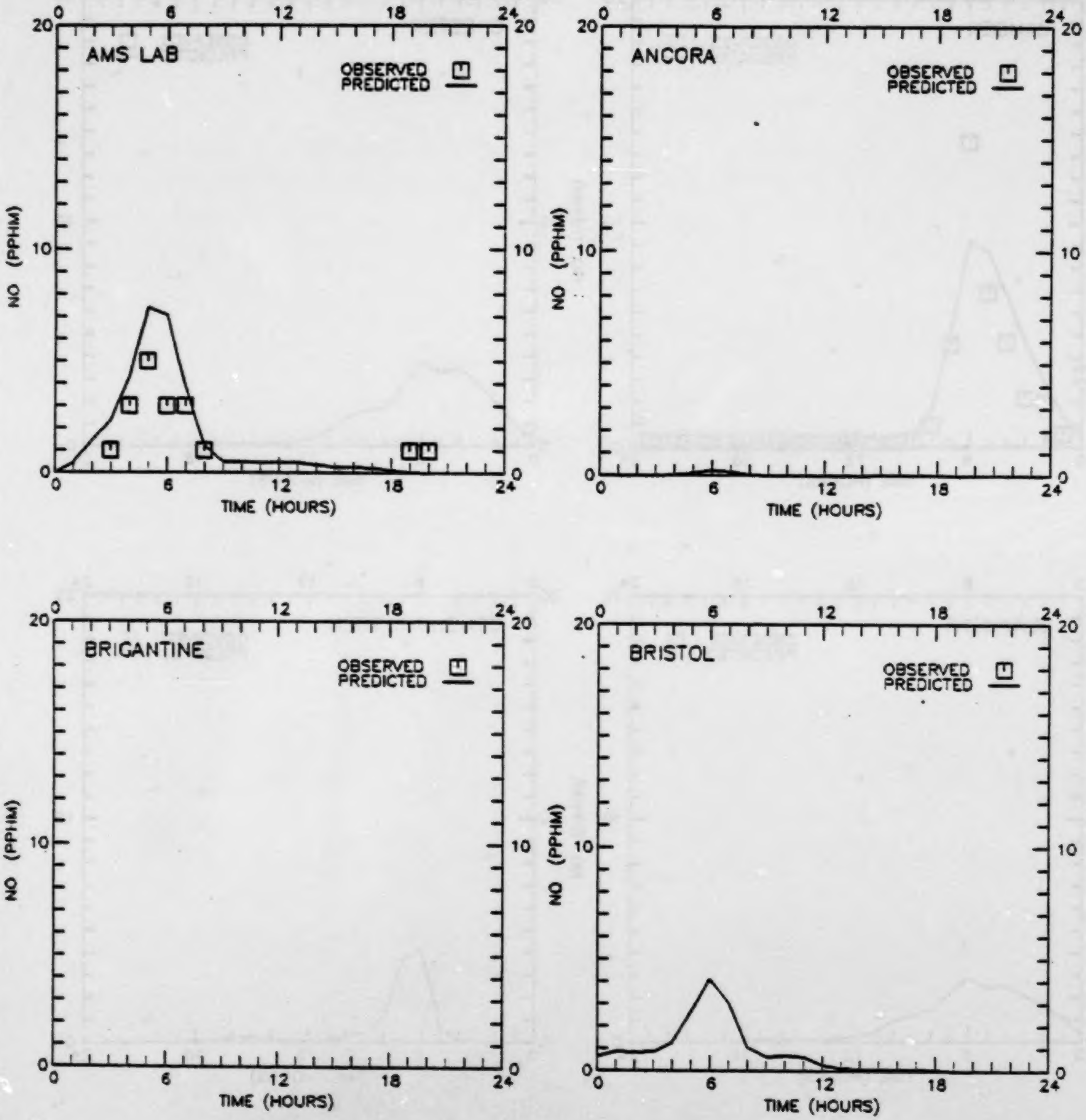
PHILADELPHIA - 7/13/79 - OZ - EVALUATION RUN



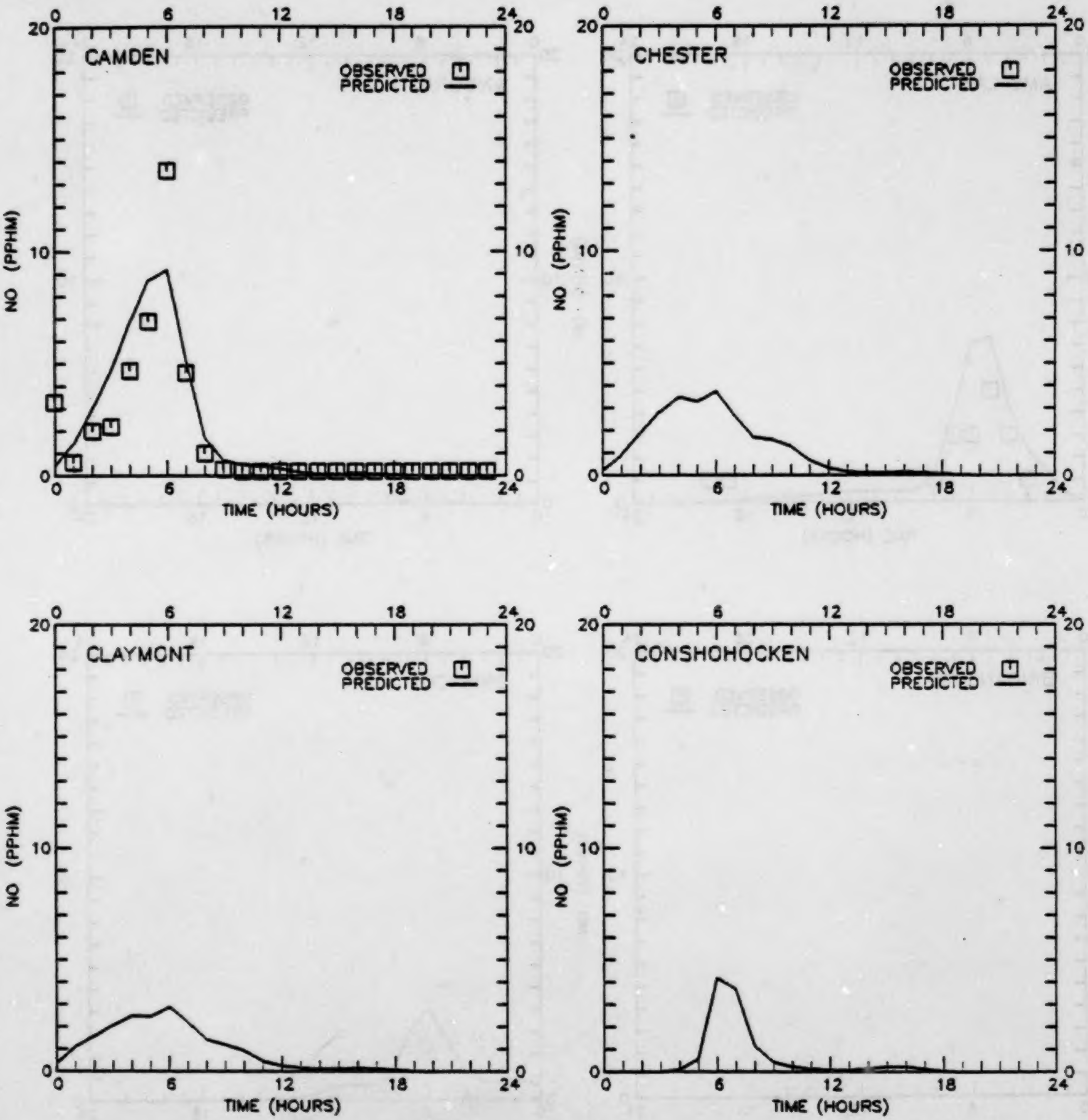
PHILADELPHIA – 7/13/79 – OZ – EVALUATION RUN



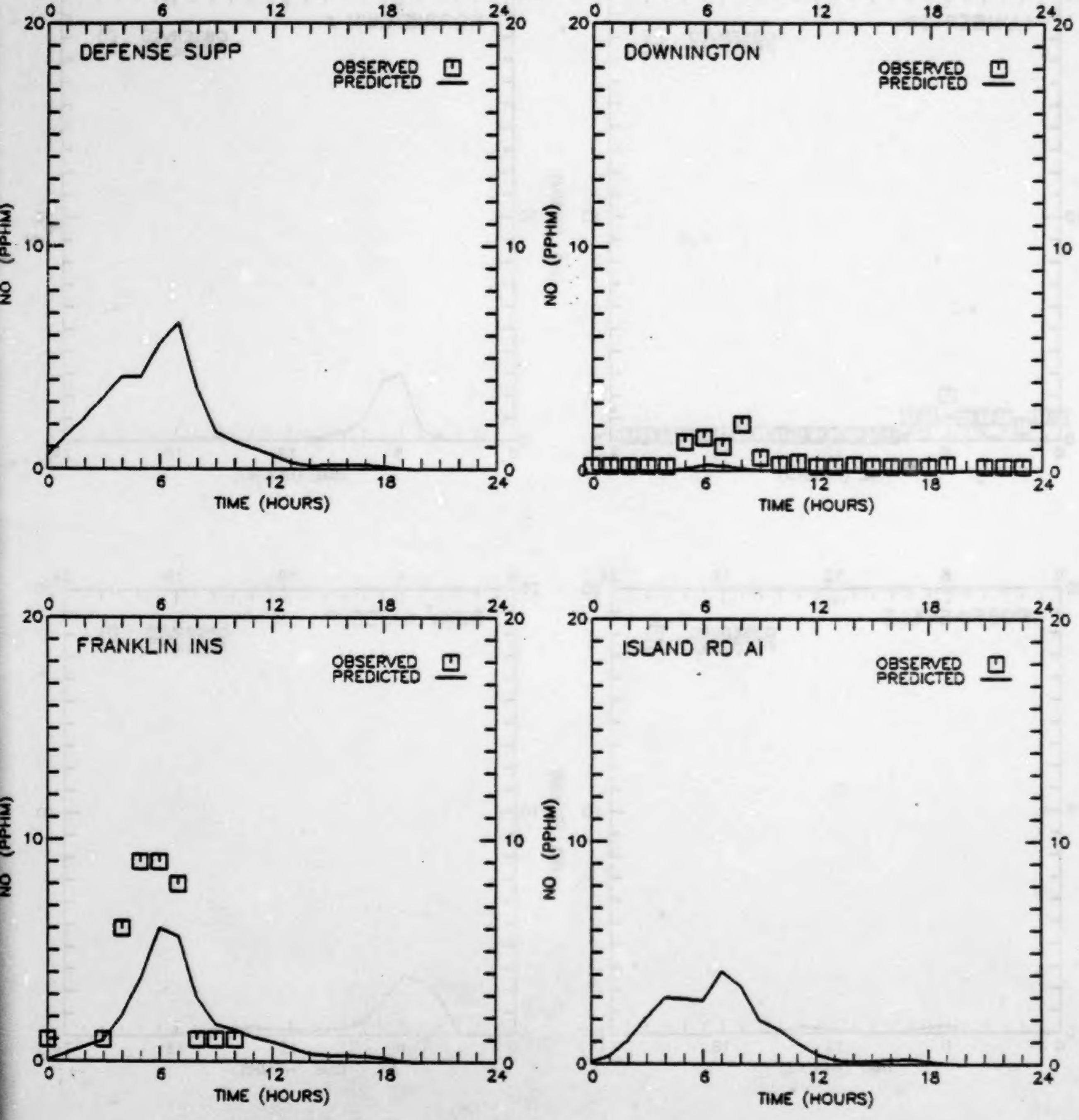
PHILADELPHIA – 7/13/79 – OZ – EVALUATION RUN



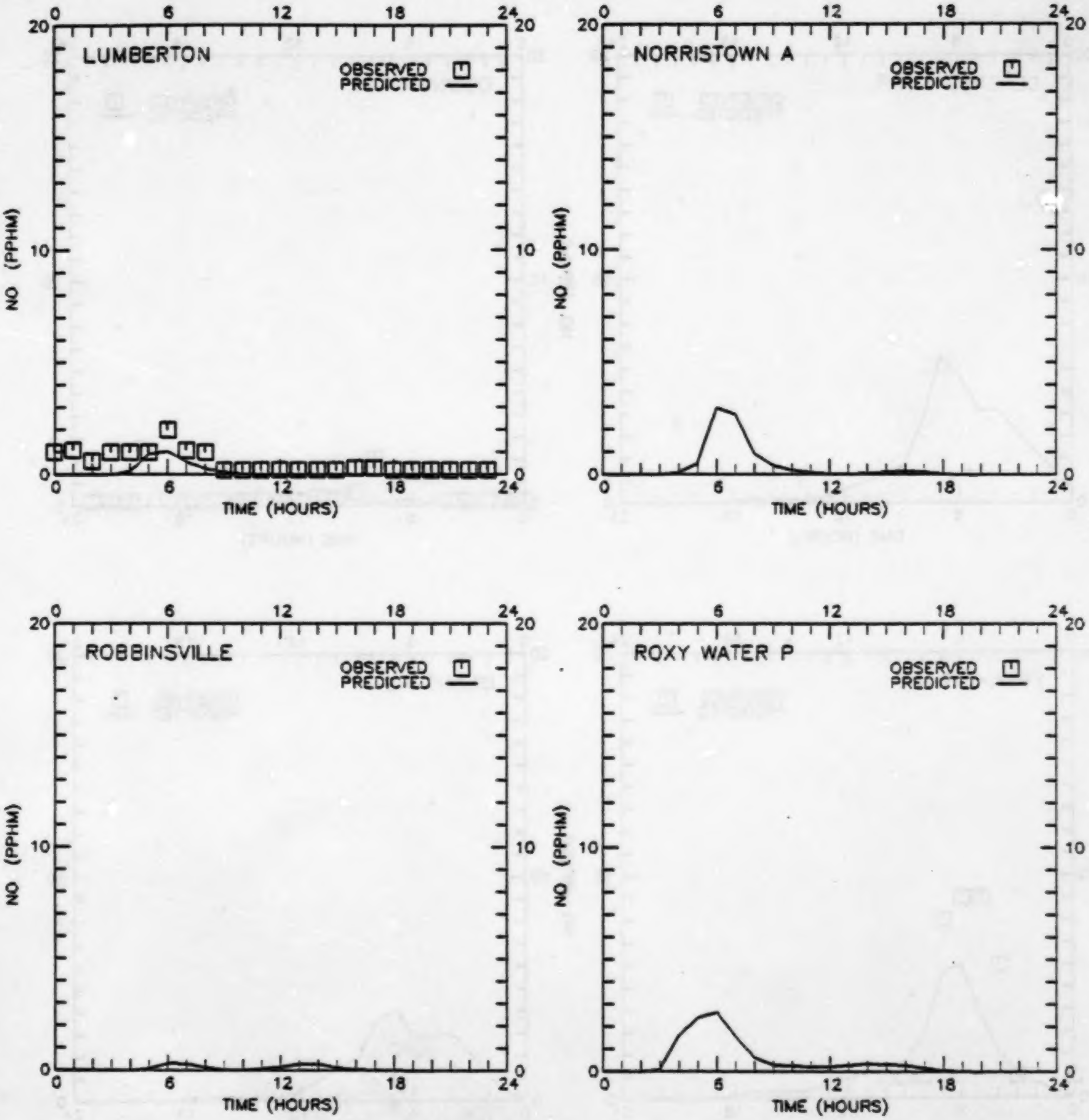
PHILADELPHIA – 7/13/79 – NO – EVALUATION RUN



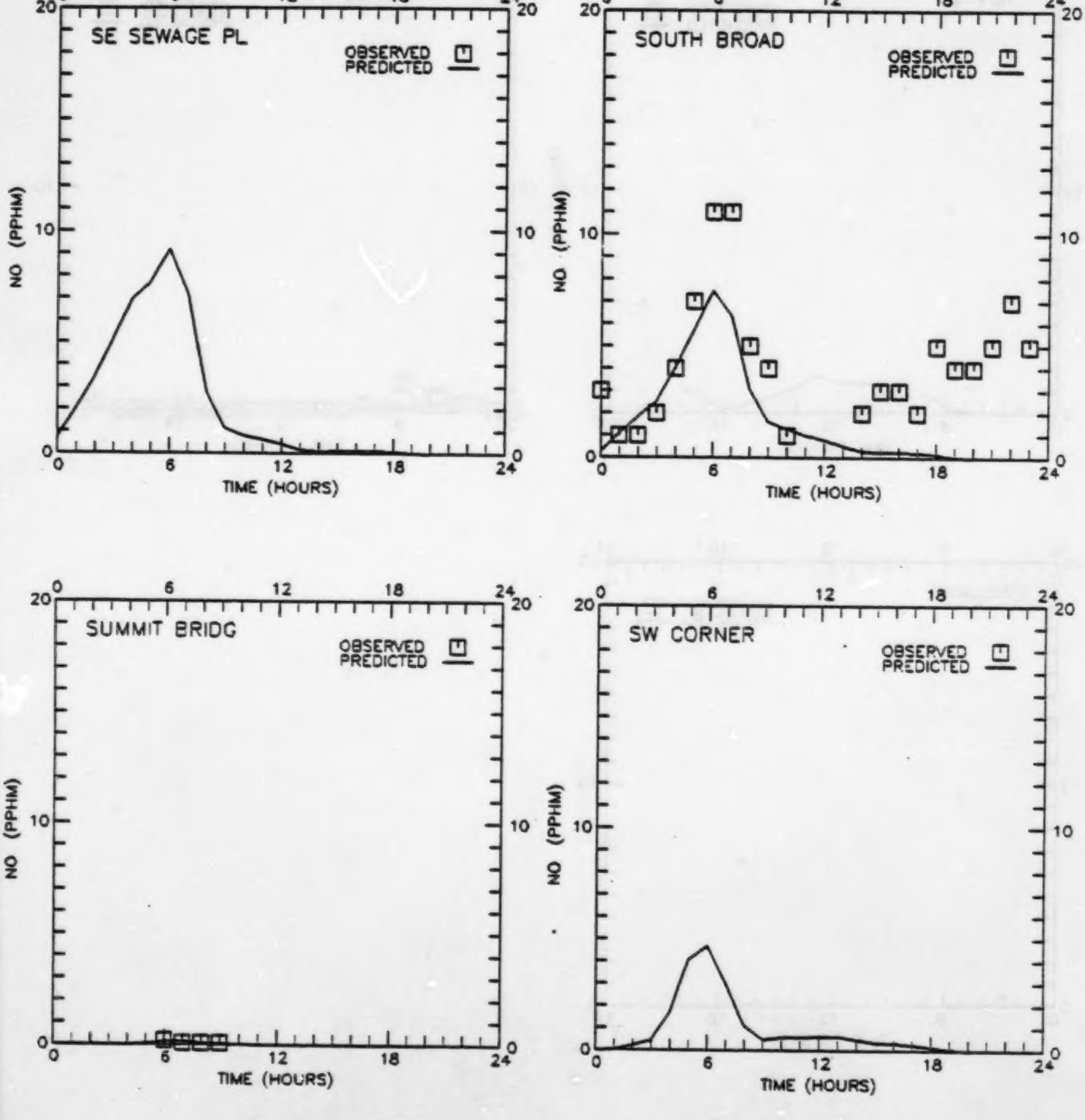
PHILADELPHIA – 7/13/79 – NO – EVALUATION RUN



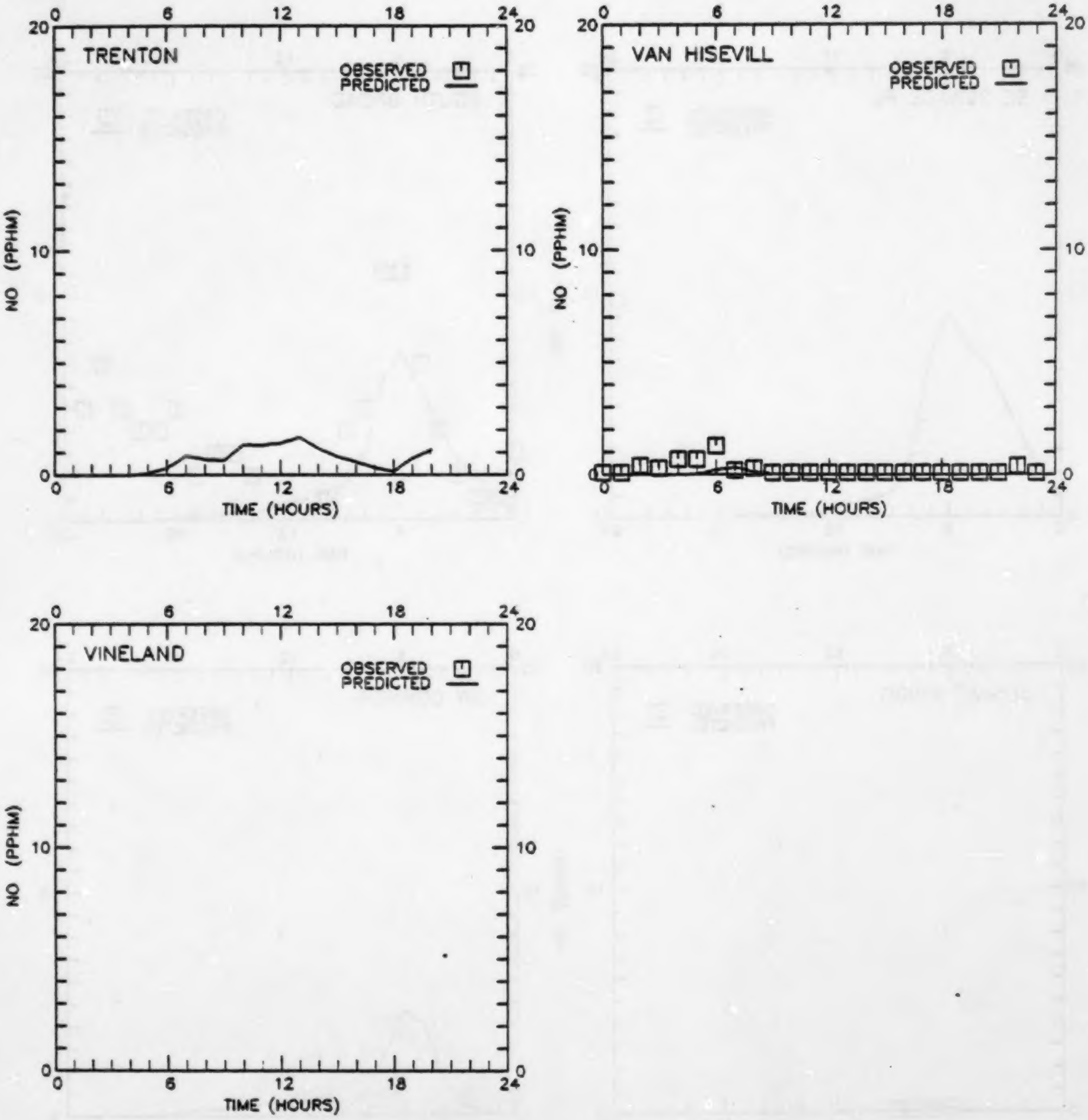
PHILADELPHIA – 7/13/79 – NO – EVALUATION RUN



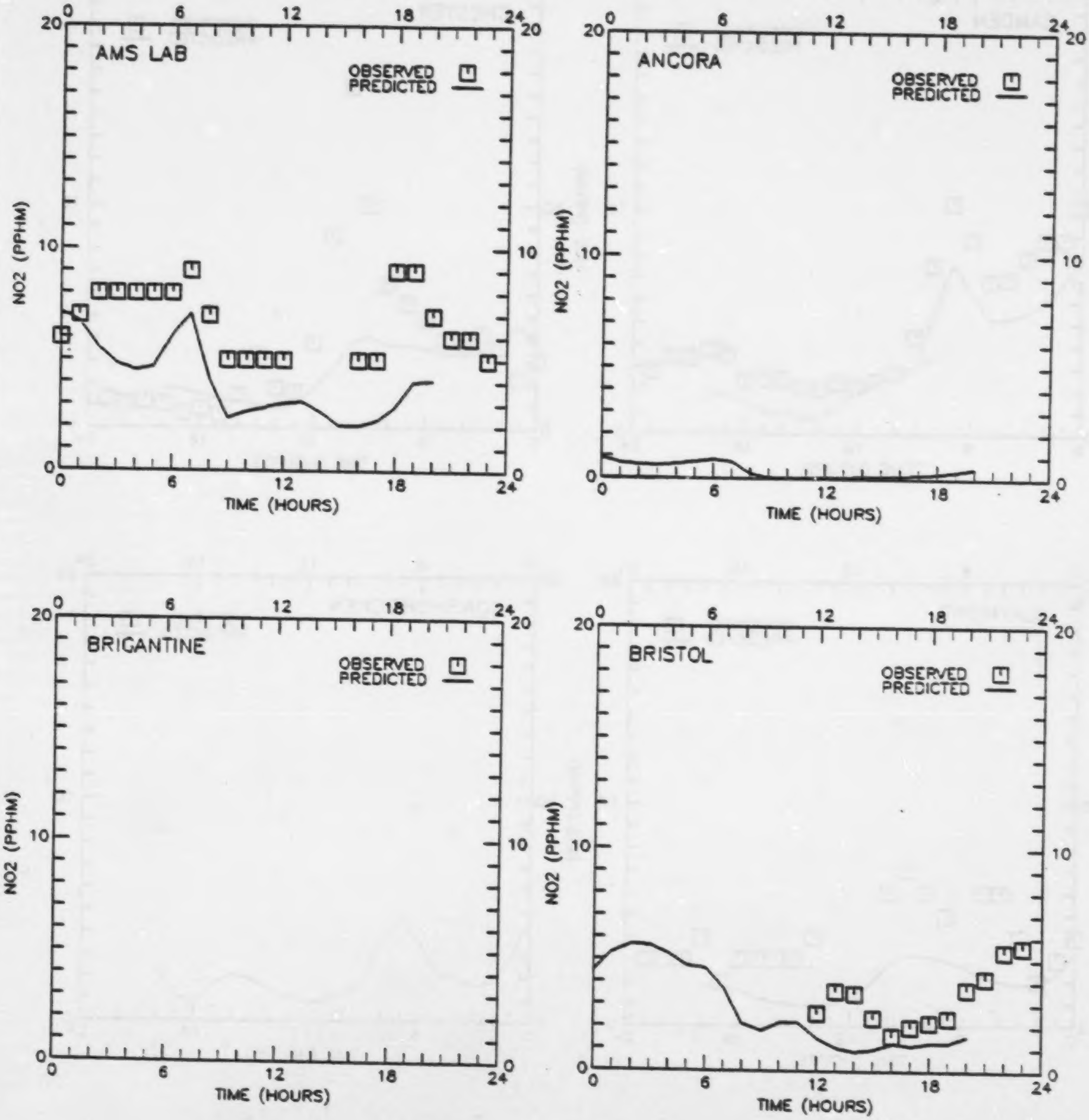
PHILADELPHIA – 7/13/79 – NO – EVALUATION RUN



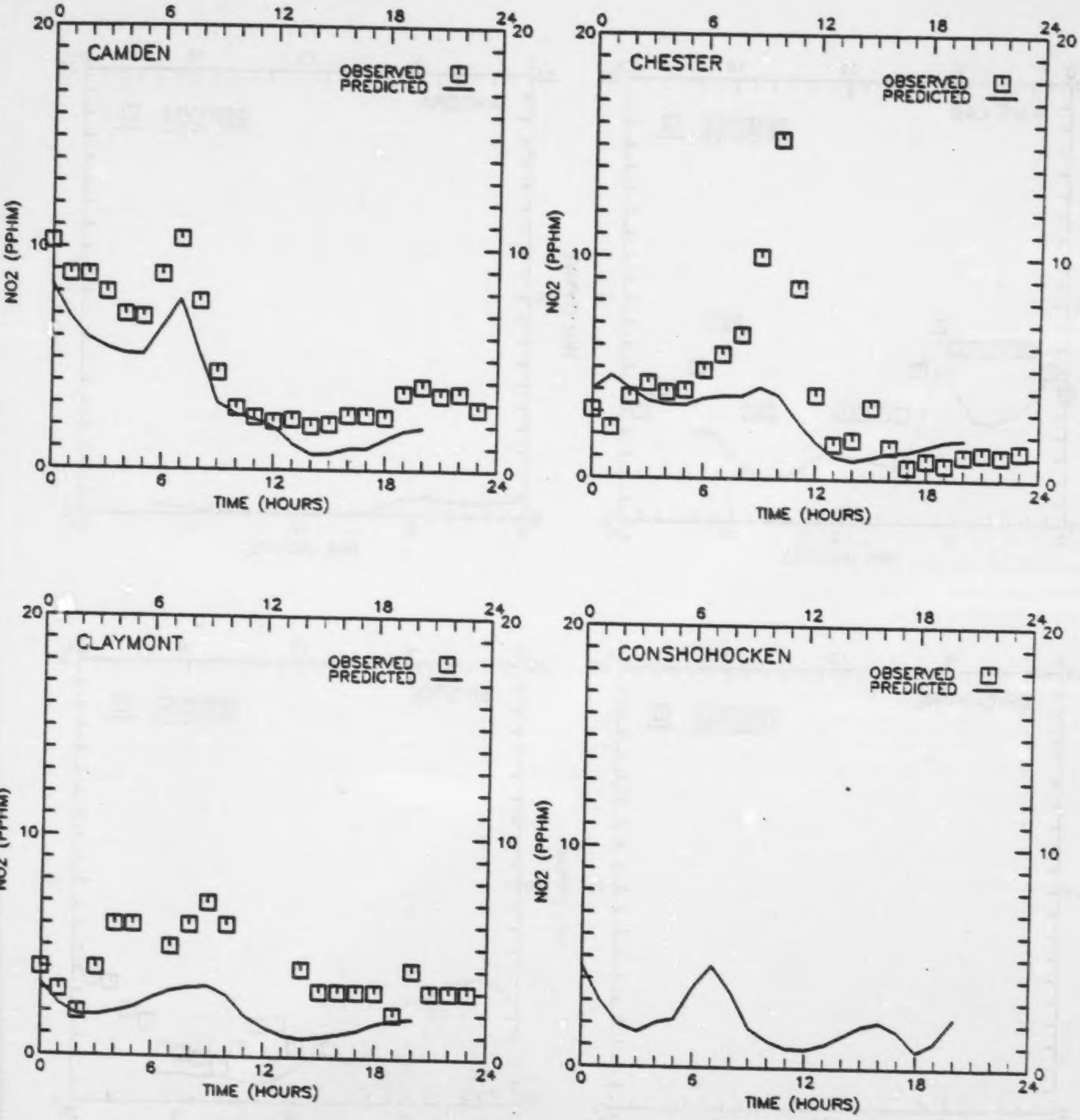
PHILADELPHIA – 7/13/79 – NO – EVALUATION RUN



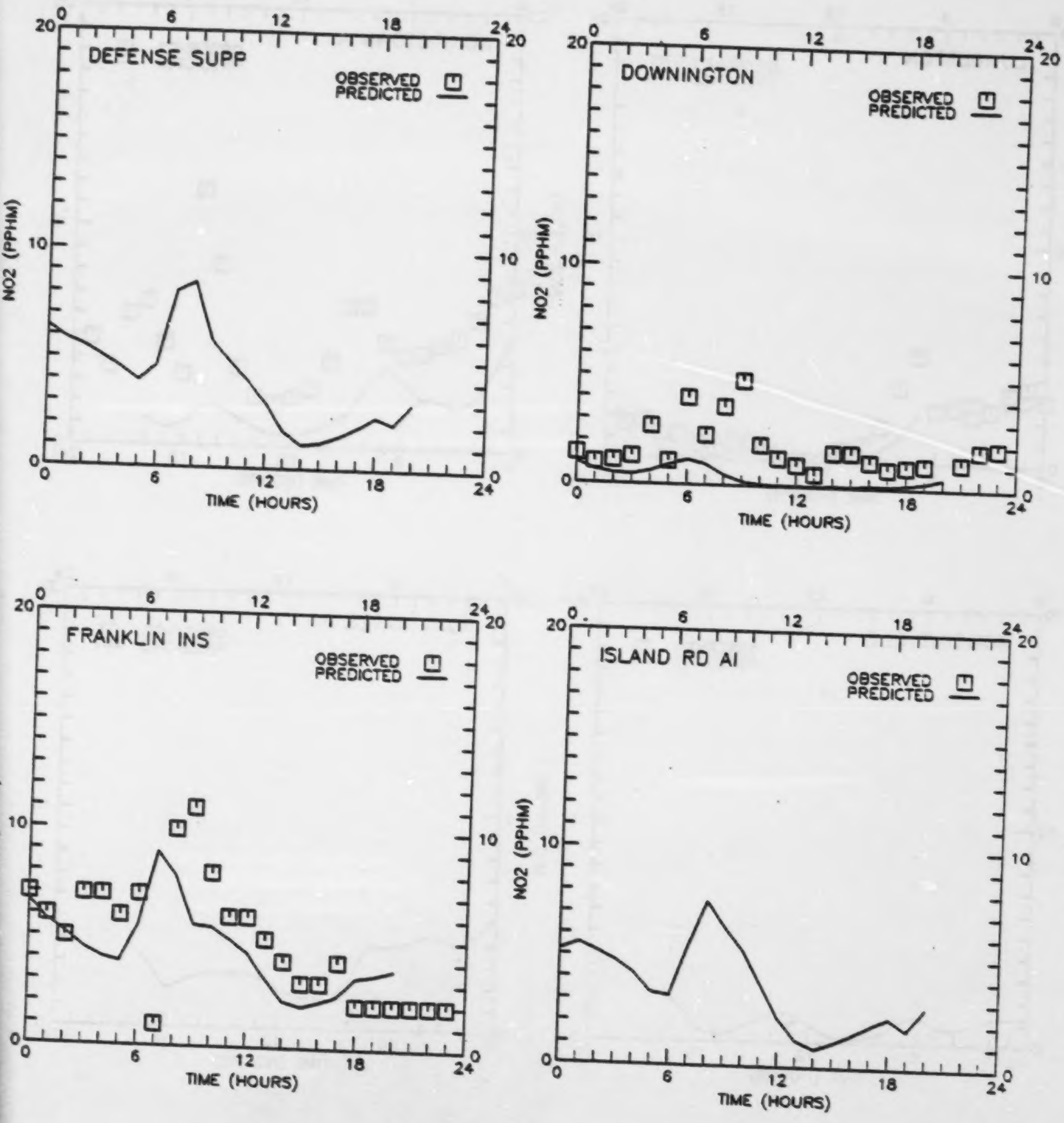
PHILADELPHIA – 7/13/79 – NO – EVALUATION RUN



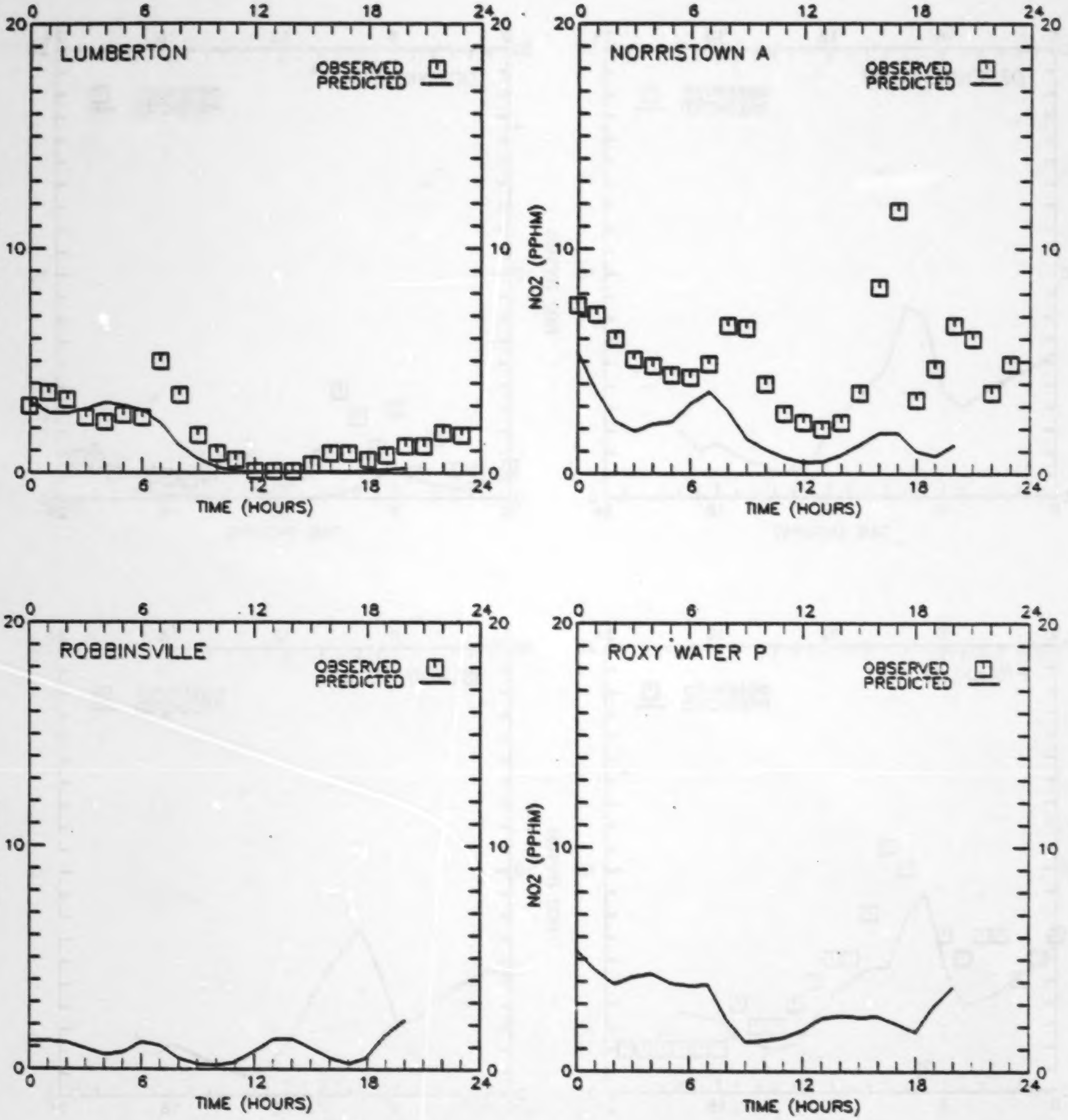
PHILADELPHIA - 7/13/79 - NO2 - EVALUATION RUN



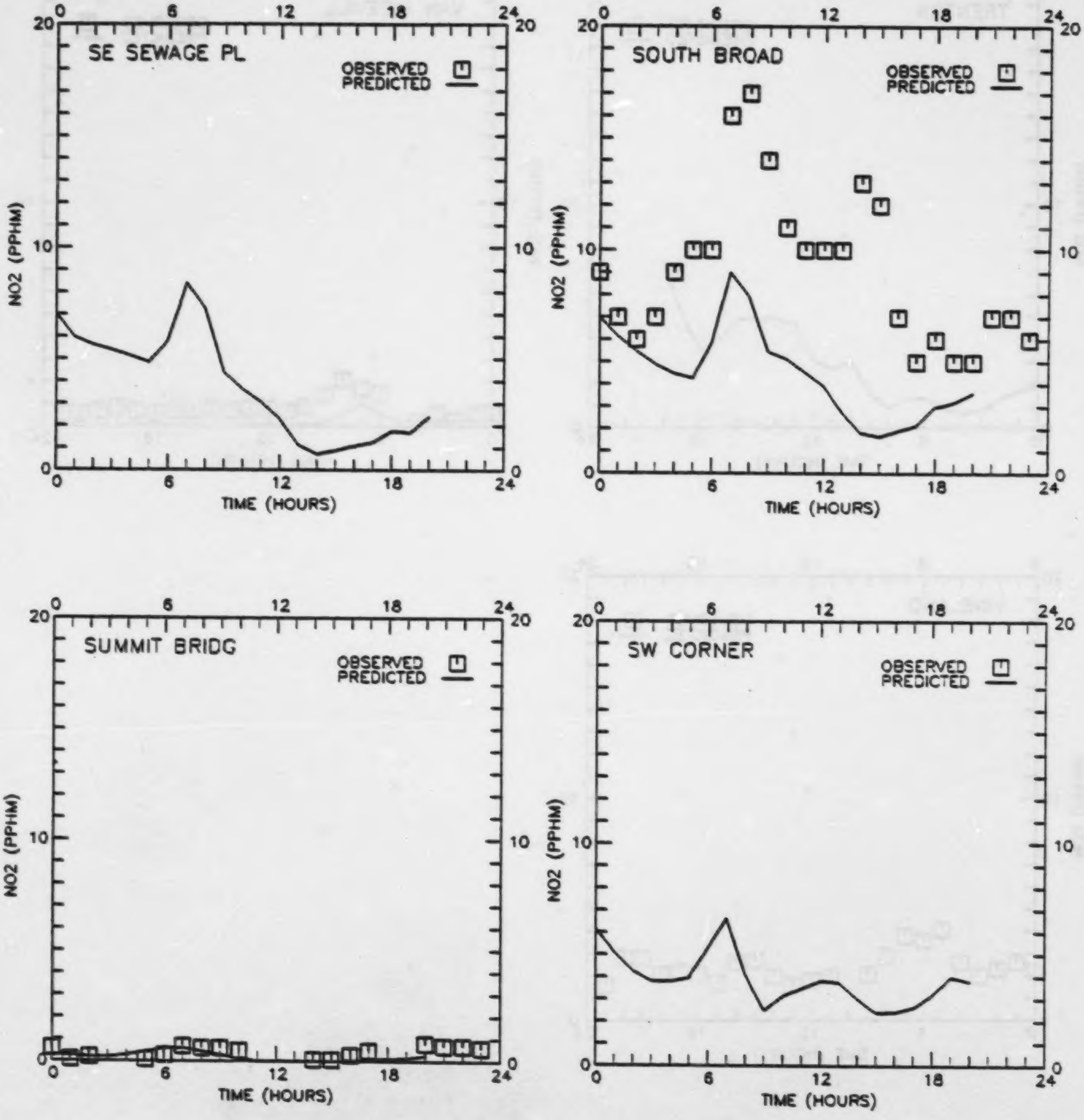
PHILADELPHIA – 7/13/79 – NO2 – EVALUATION RUN



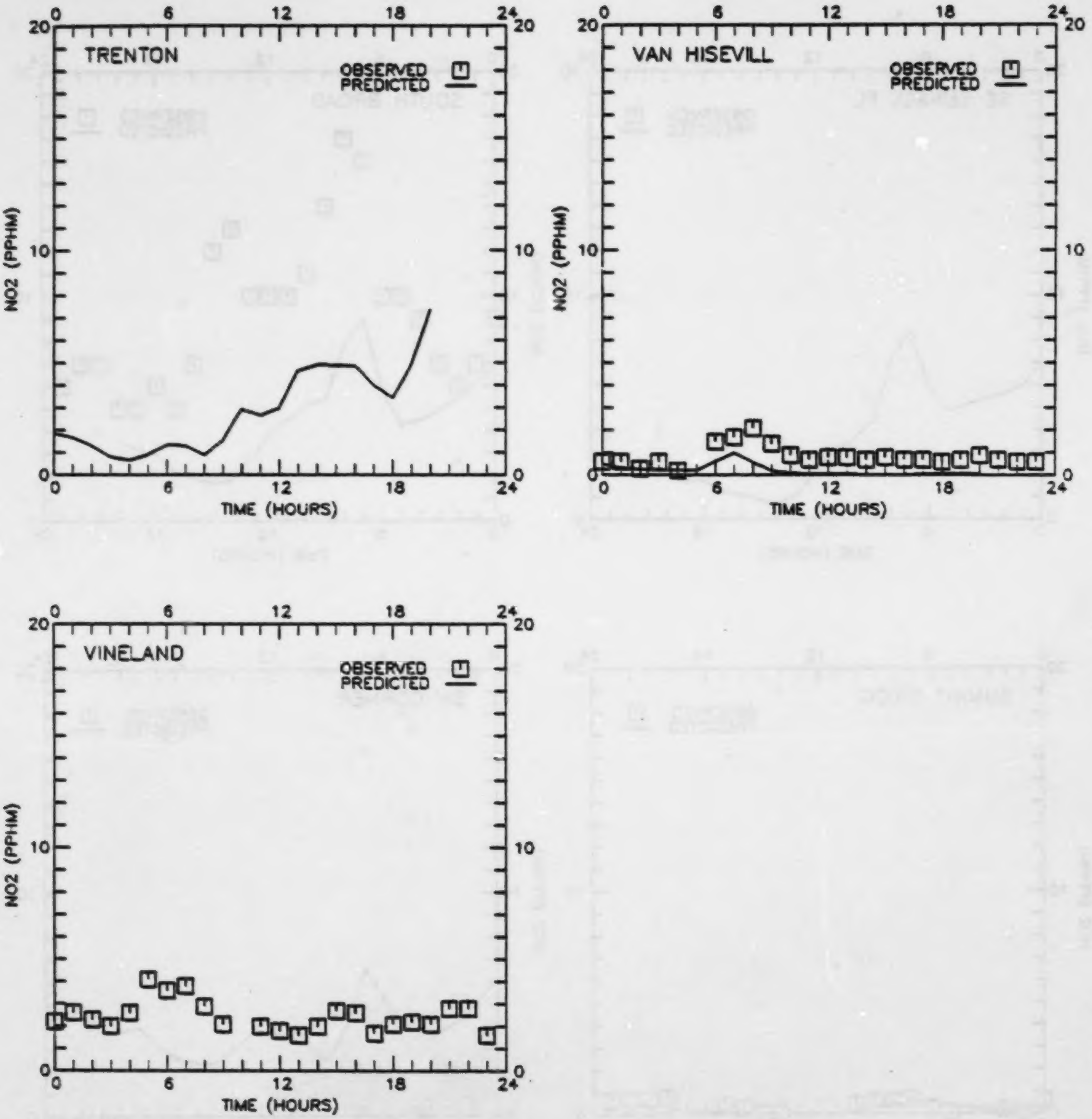
PHILADELPHIA – 7/13/79 – NO2 – EVALUATION RUN



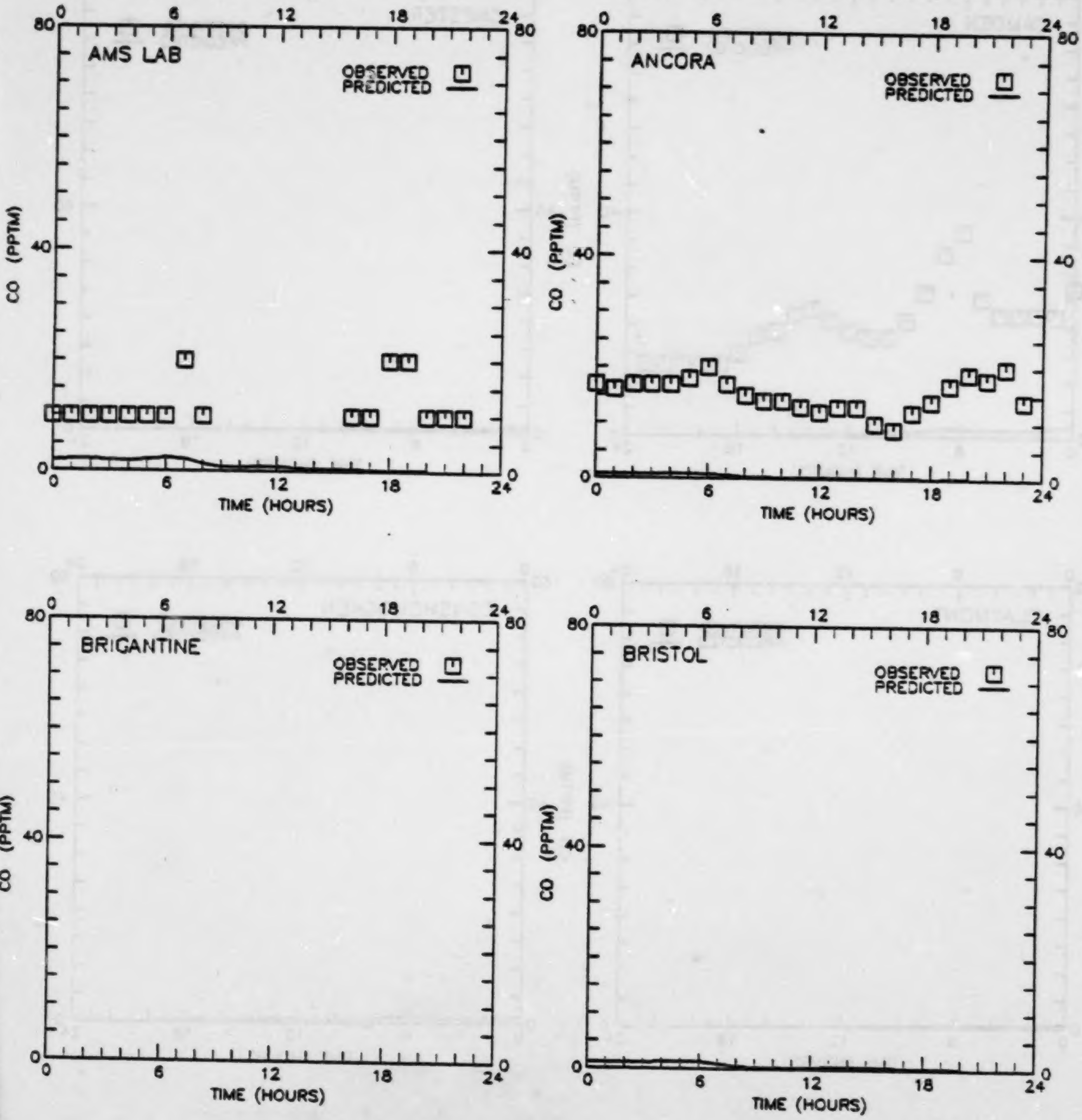
PHILADELPHIA – 7/13/79 – NO2 – EVALUATION RUN



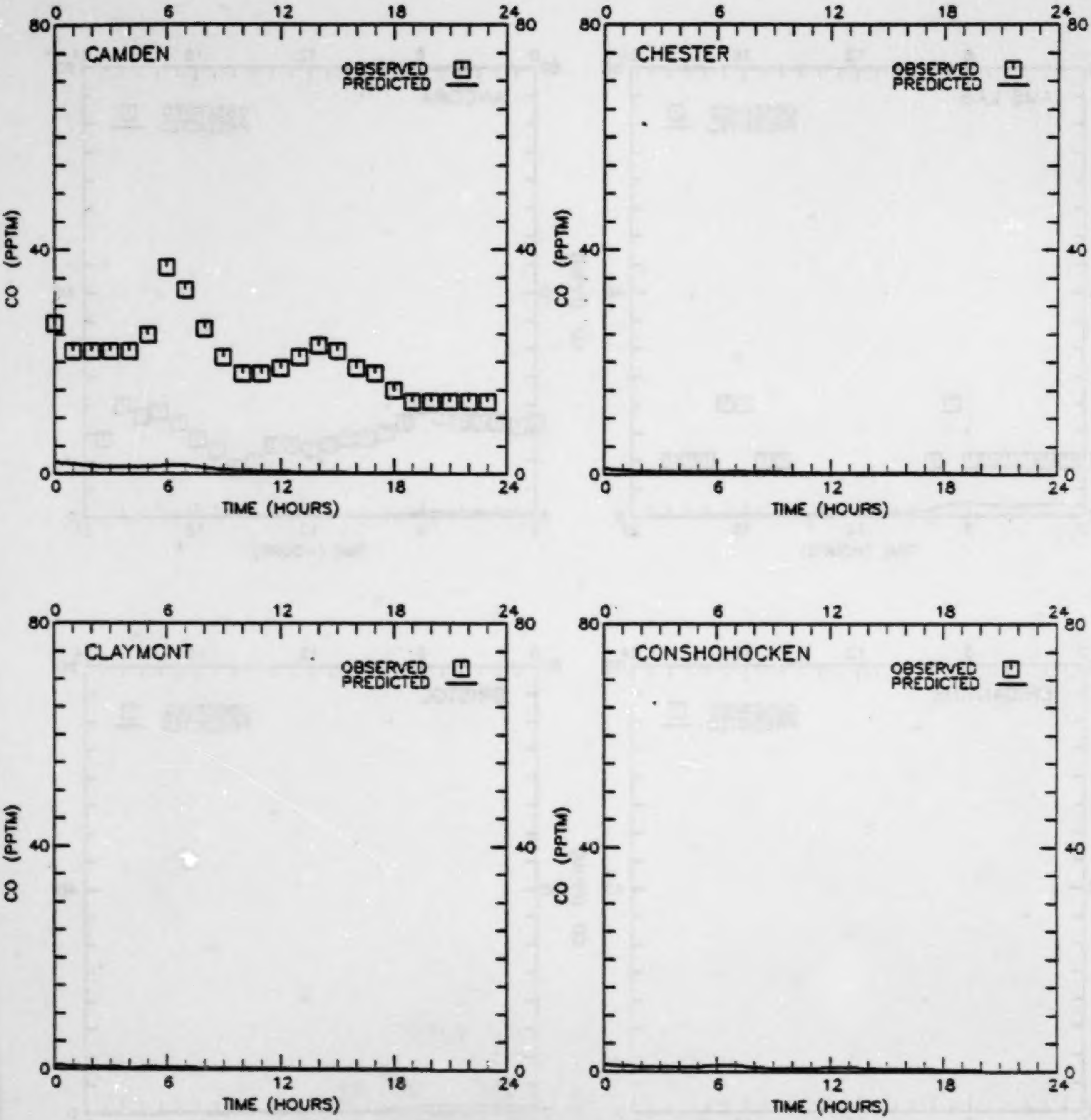
PHILADELPHIA – 7/13/79 – NO2 – EVALUATION RUN



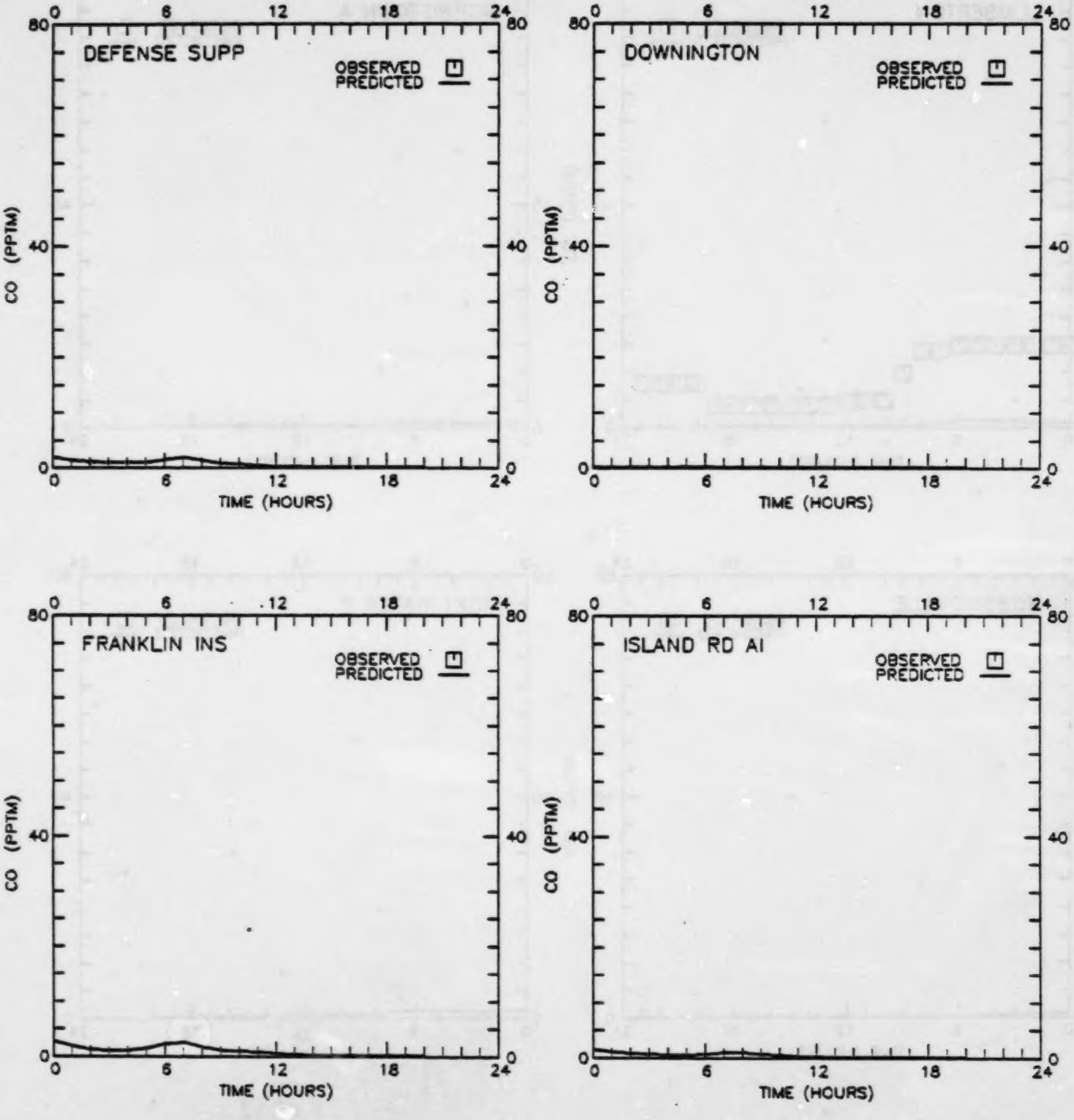
PHILADELPHIA – 7/13/79 – NO2 – EVALUATION RUN



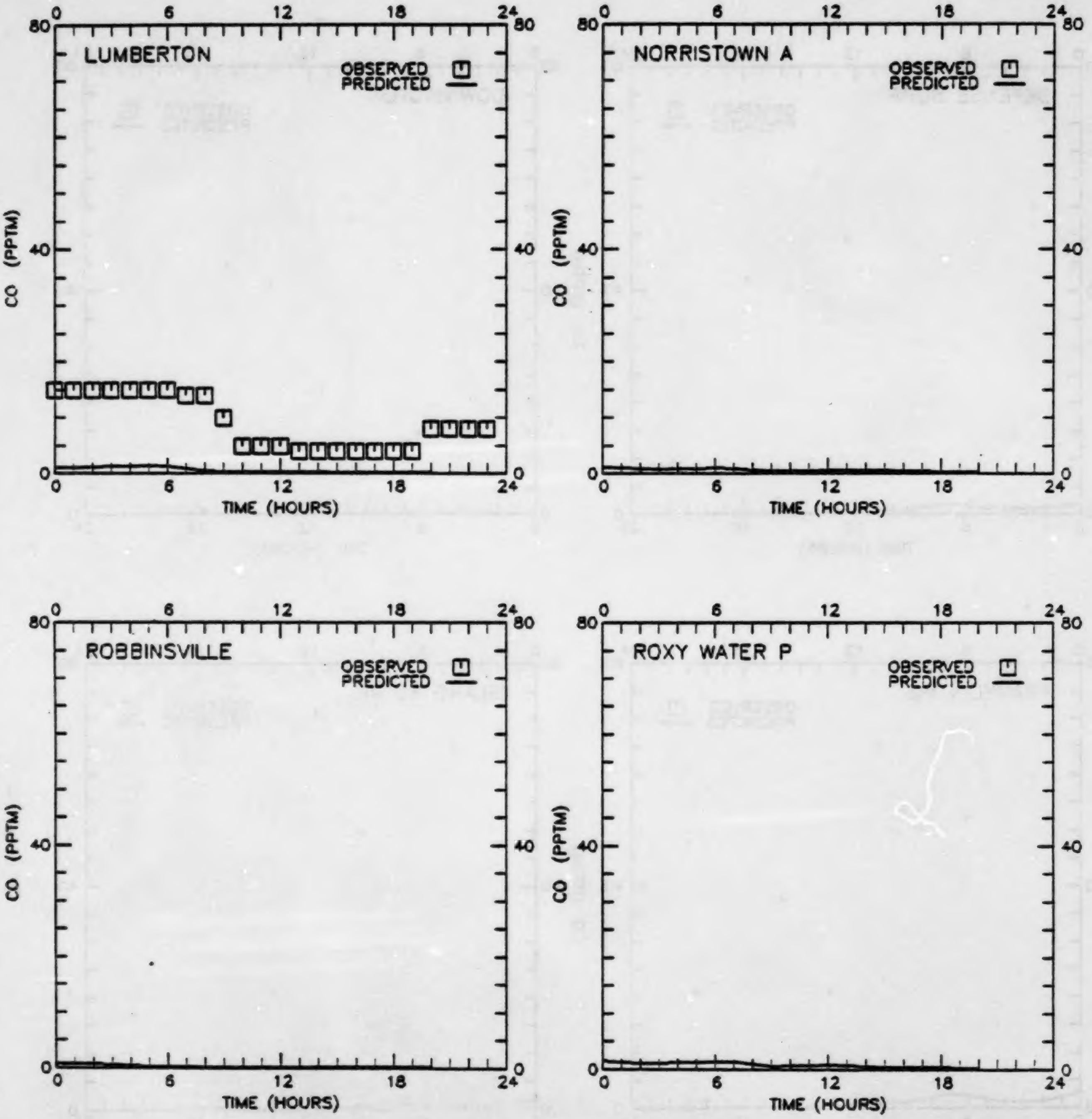
PHILADELPHIA – 7/13/79 – CO – EVALUATION RUN



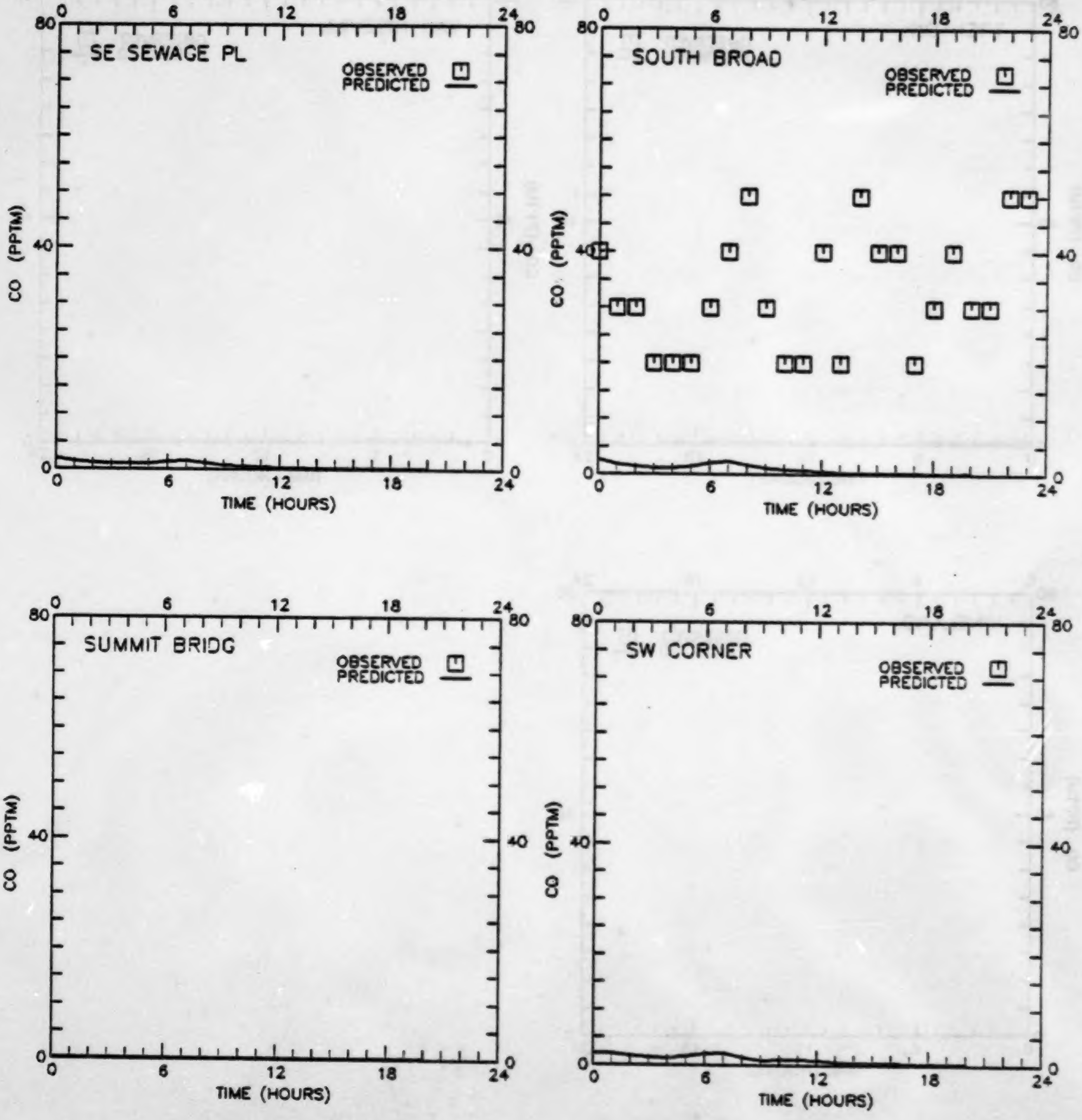
PHILADELPHIA – 7/13/79 – CO – EVALUATION RUN



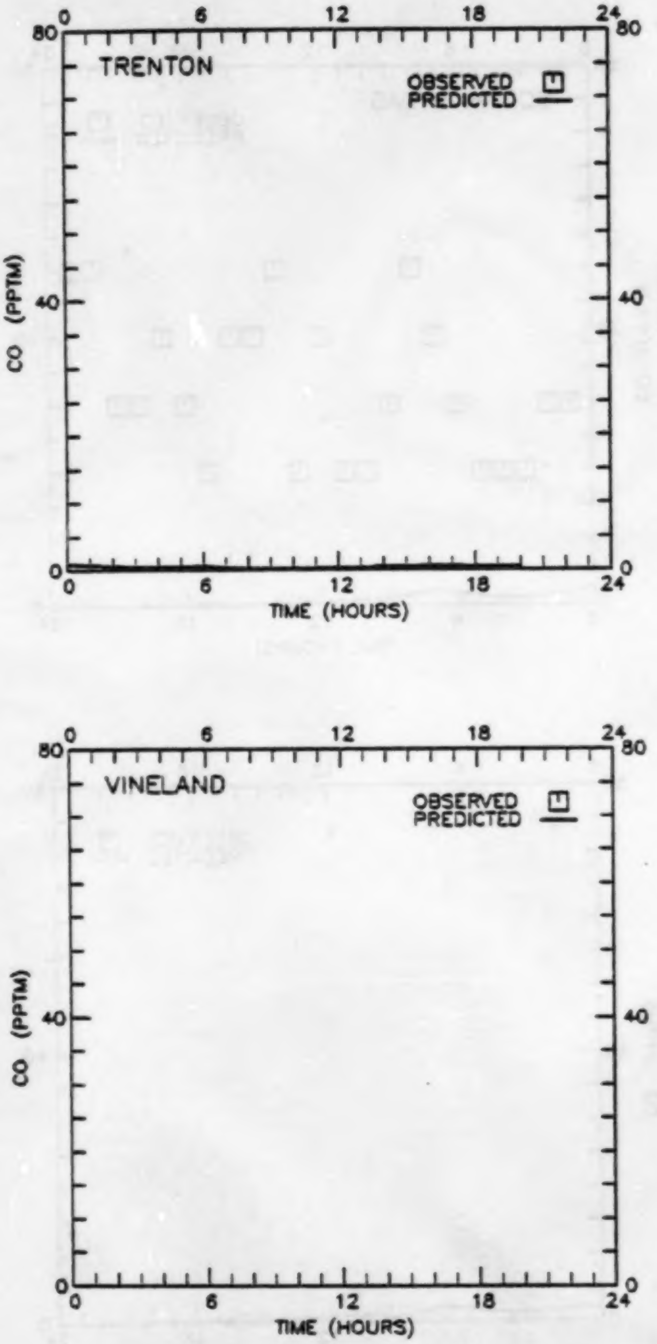
PHILADELPHIA – 7/13/79 – CO – EVALUATION RUN



PHILADELPHIA – 7/13/79 – CO – EVALUATION RUN



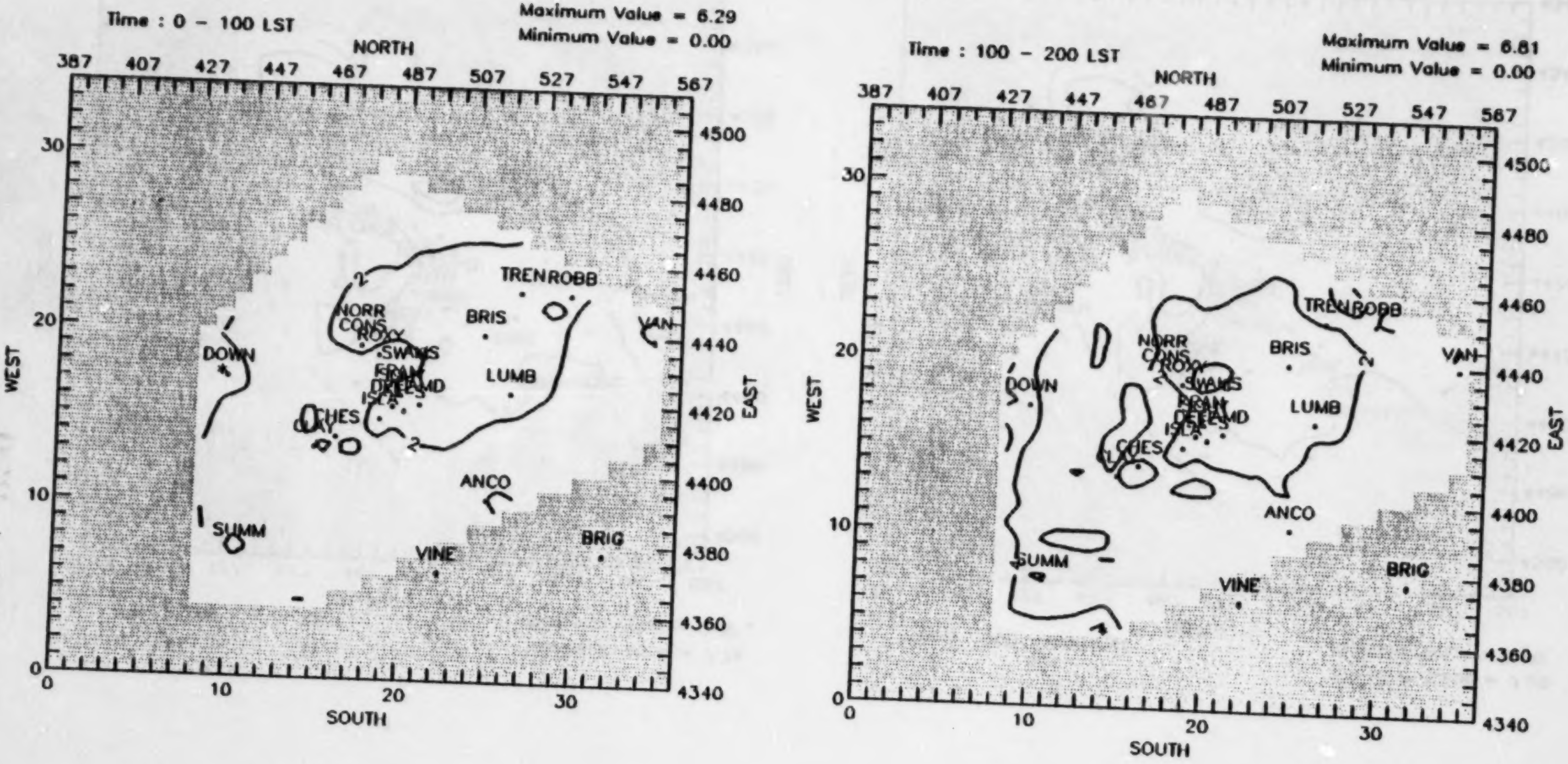
PHILADELPHIA – 7/13/79 – CO – EVALUATION RUN (SIMPLE)



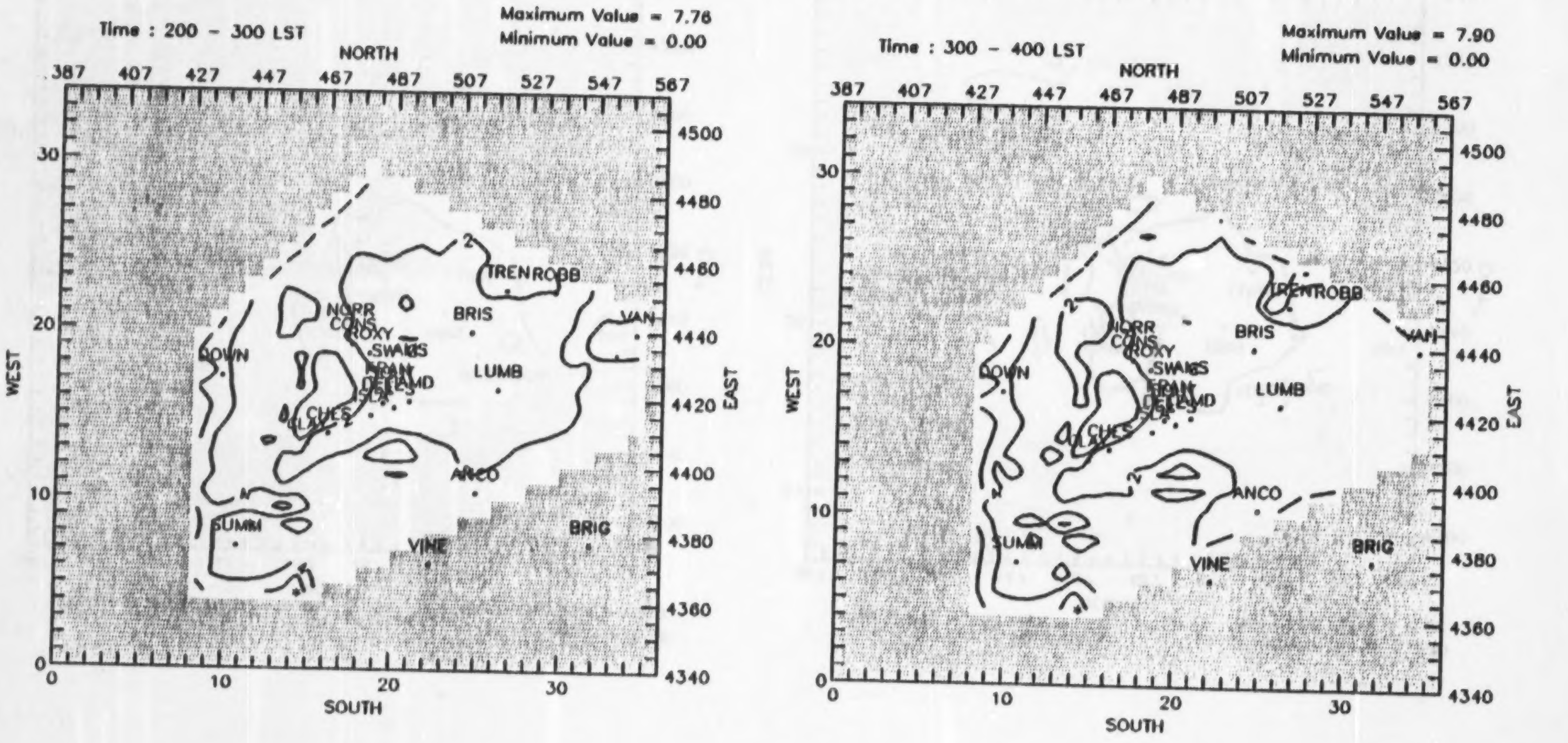
PHILADELPHIA – 7/13/79 – CO – EVALUATION RUN

Appendix H

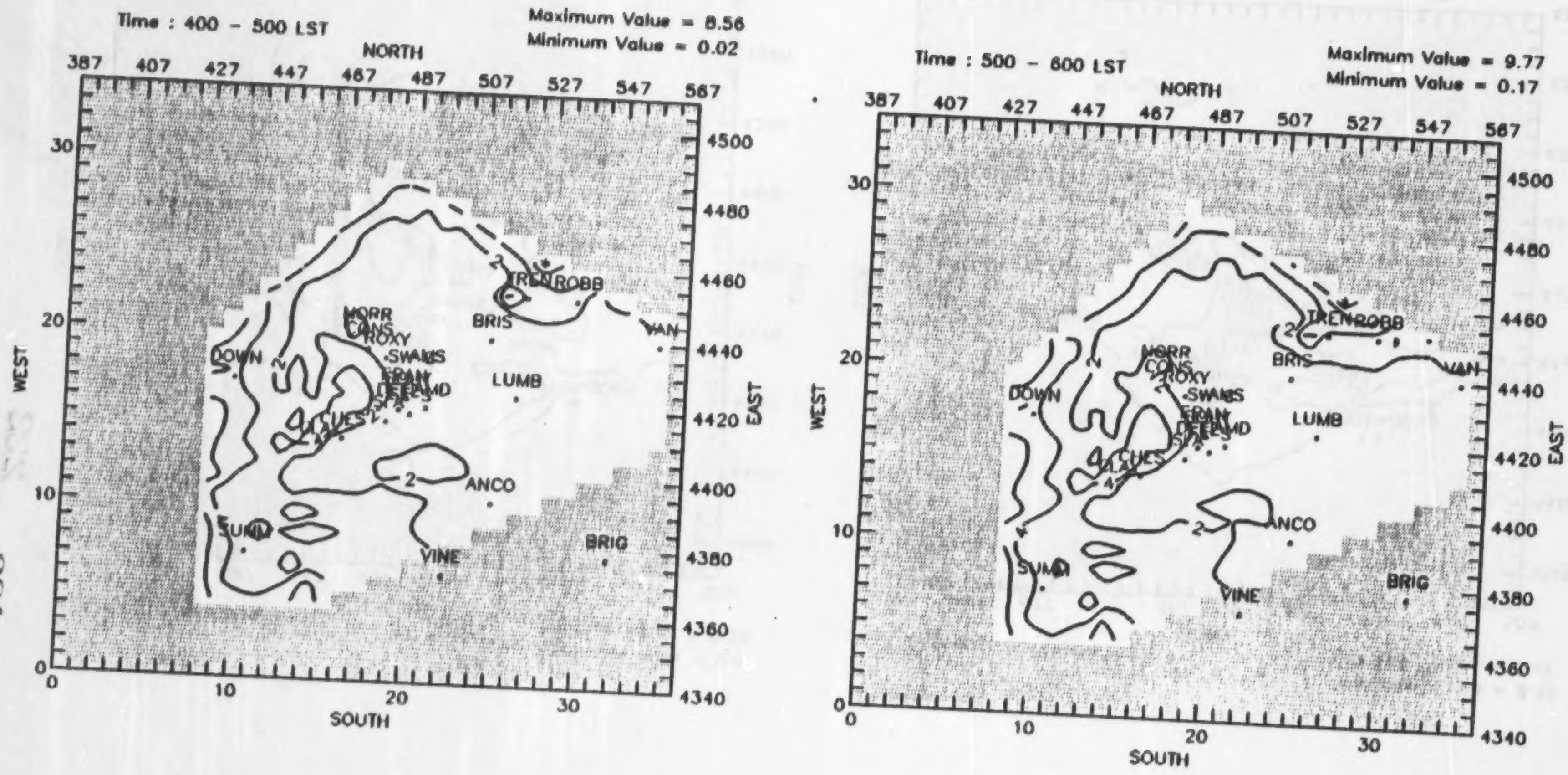
HOURLY OZONE CONCENTRATIONS (pphm) IN PHILADELPHIA PREDICTED BY THE UAM(CB-IV) USING A RICH DATA BASE (POS UAM)


Time : 0 - 100 LST
Maximum Value = 6.29
Minimum Value = 0.00
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
0
10
20
30
4340
4360
4380
4400
4420
4440
4460
4480
4500
TRENROBB
NORR
CONS
ROXY
SWANS
FRAN
DEFEAMD
ISLA
CHES
CLAY
BRIS
LUMB
DOWN
VAN
ANCO
SUMM
VINE
BRIG
2
Time : 100 - 200 LST
Maximum Value = 6.81
Minimum Value = 0.00

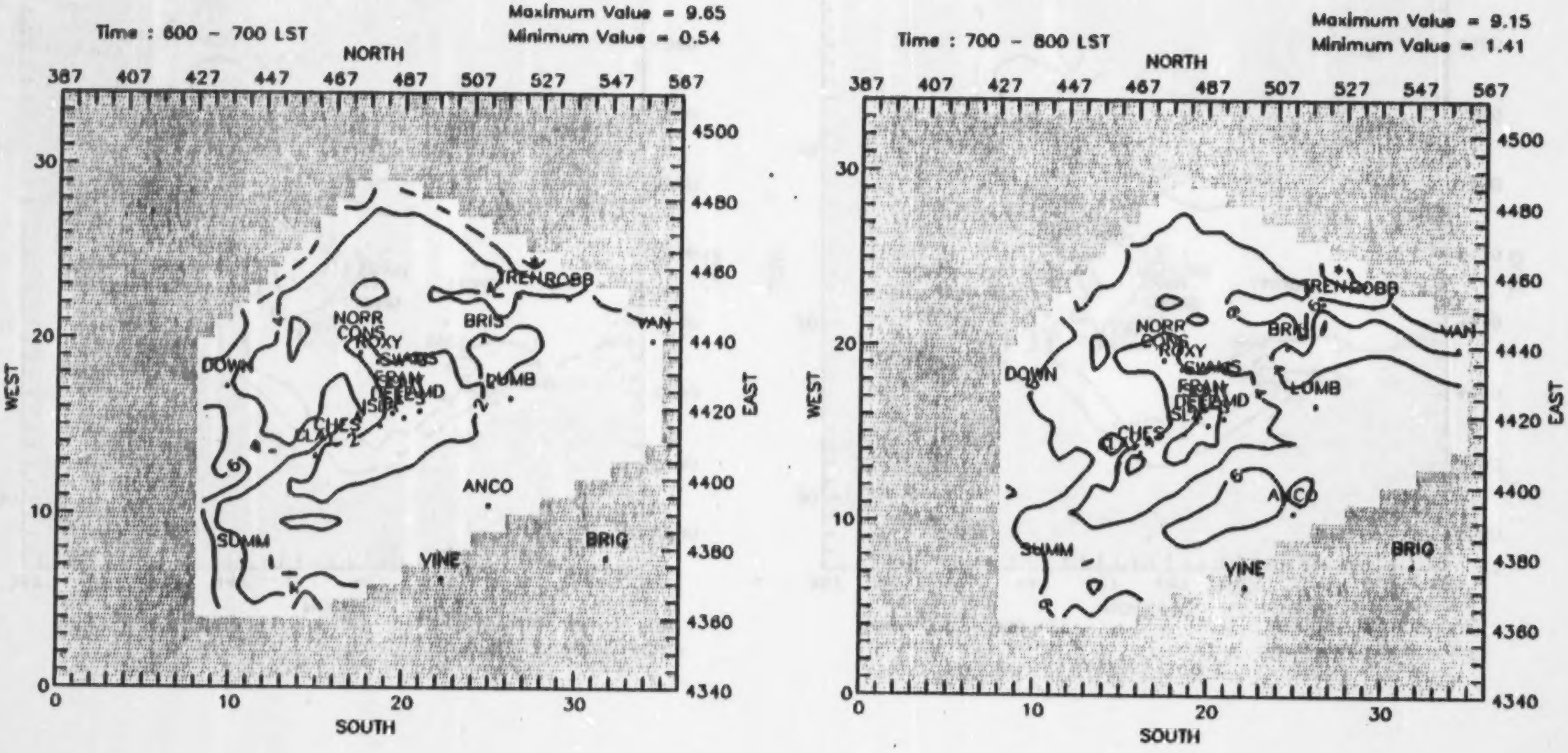
Ozone (pphm) 1979 base emissions, July 13, 1979 (pacr1)


Time : 200 - 300 LST
Maximum Value = 7.76
Minimum Value = 0.00
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
NORR
CONS
ROXY
SWAIS
FRAN
DETLMD
SLS
CHES
CLAY
BRIS
LUMB
DOWN
VAN
ANCO
SUMM
VINE
BRIG
2
Time : 300 - 400 LST
Maximum Value = 7.90
Minimum Value = 0.00

Ozone (pphm) 1979 base emissions, July 13, 1979 (pacr1)


Time : 400 - 500 LST
Maximum Value = 8.56
Minimum Value = 0.02
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
0
10
20
30
4340
4360
4380
4400
4420
4440
4460
4480
4500
TREN
ROBB
NORR
CONS
ROXY
BRIS
VAN
DOWN
SWANS
FRAN
DEEL
LMD
LUMB
CUES
ANCO
SUNI
VINE
BRIG
2
4
Time : 500 - 600 LST
Maximum Value = 9.77
Minimum Value = 0.17

Ozone (pphm) 1979 base emissions, July 13, 1979 (pacr1)



Time : 600 - 700 LST

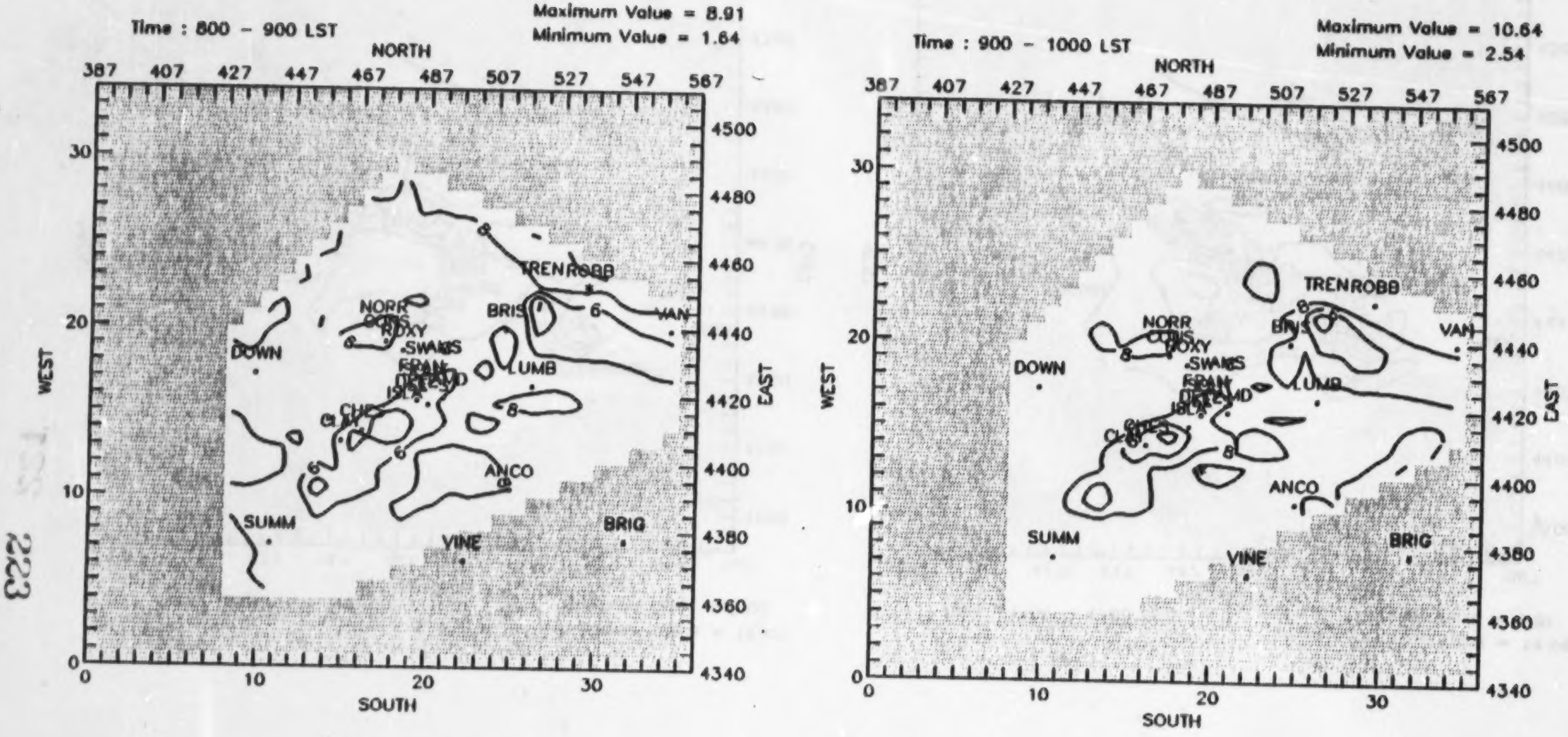
Maximum Value = 9.65
Minimum Value = 0.54

Time : 700 - 800 LST

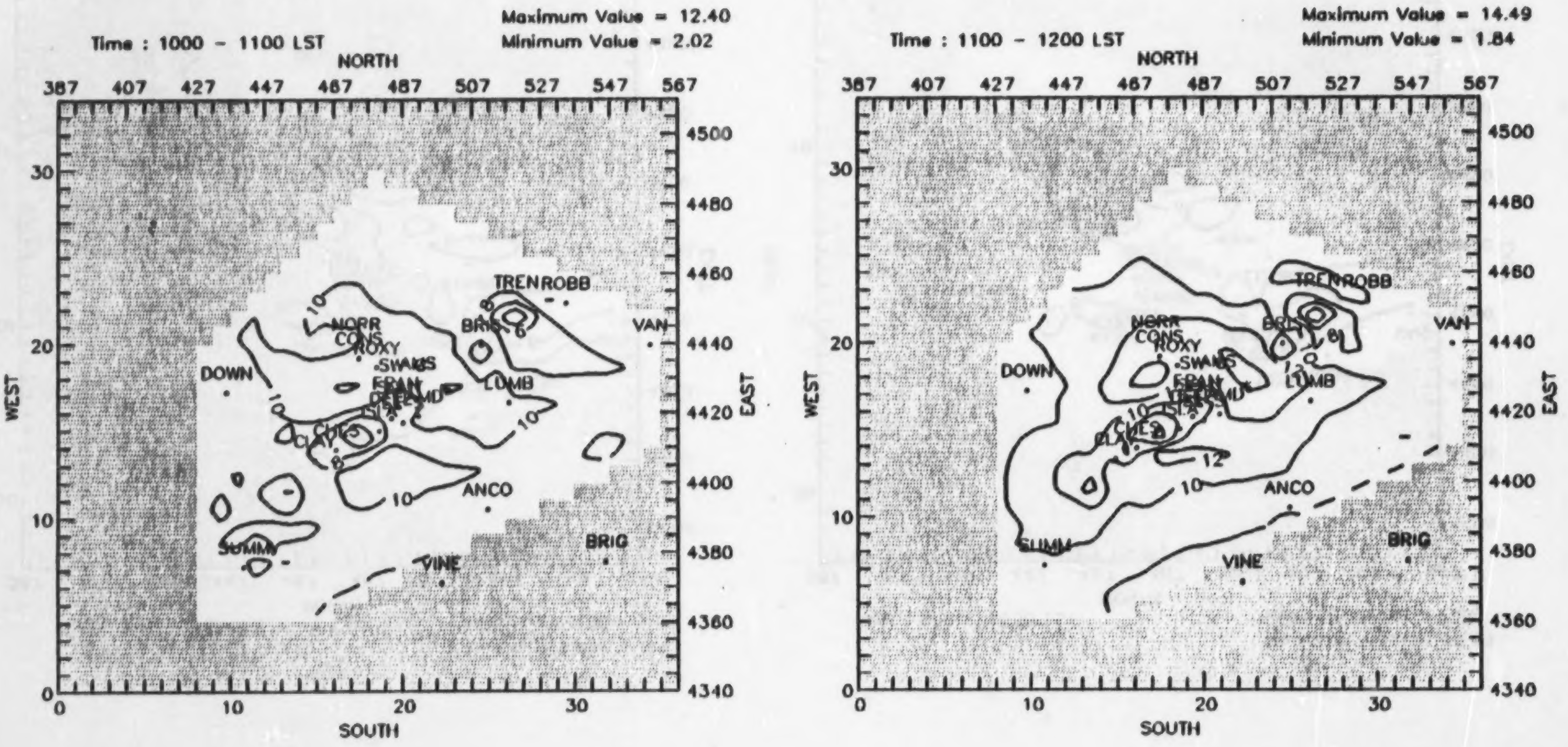
Maximum Value = 9.15
Minimum Value = 1.41

NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TREN
ROBB
VAN
BRIS
NORR
CONS
ROXY
SWAR
FRAN
DEFE
MD
DOWN
DUMB
LOMB
CHES
ANCO
SUMM
VINE
BRIG

Ozone (pphm) 1979 base emissions, July 13, 1979 (pacr1)

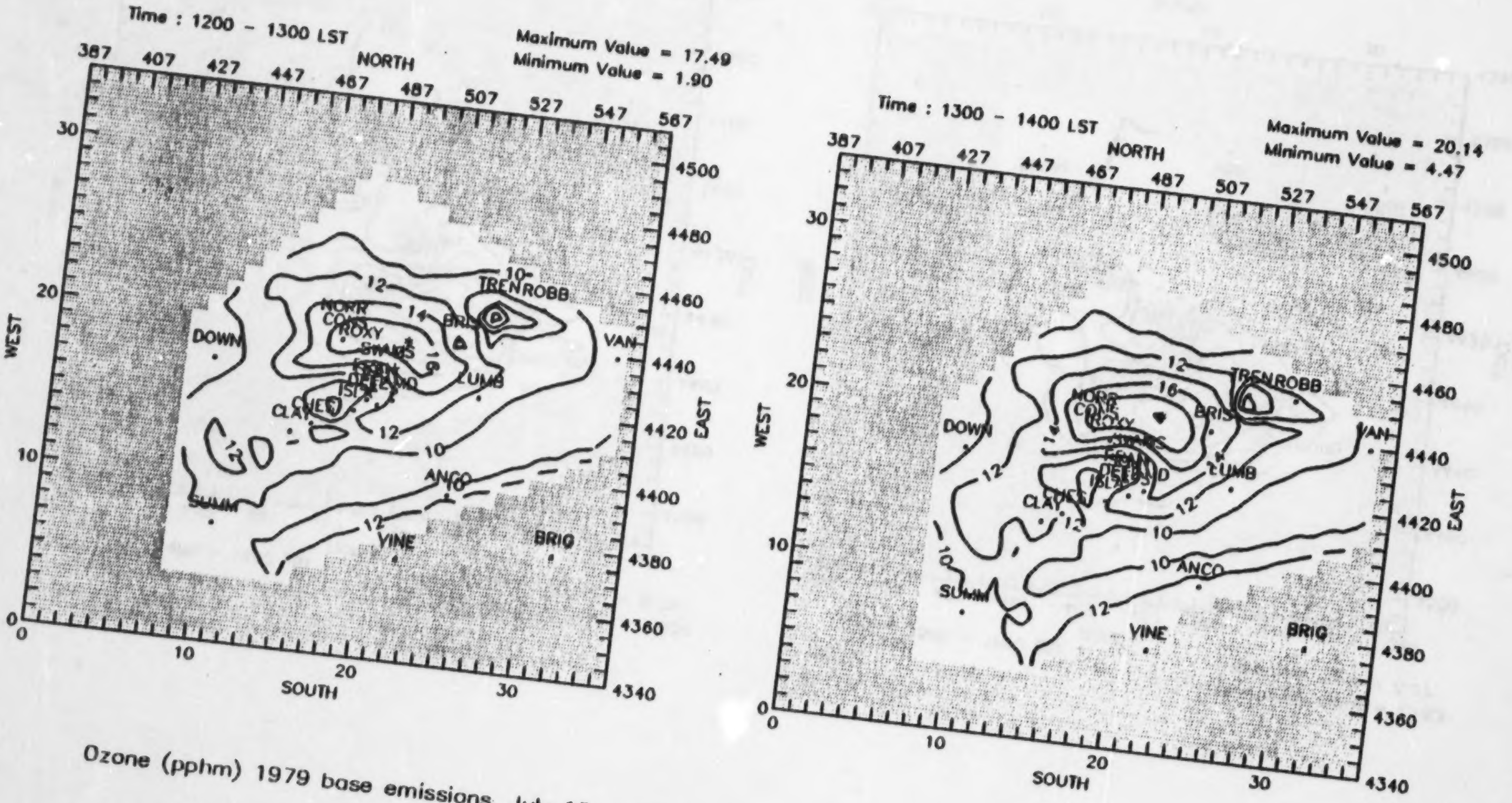

Time : 800 - 900 LST
Maximum Value = 8.91
Minimum Value = 1.64
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
BRIS
VAN
NORR
ROXY
SWANS
FRAN
LUMB
CHE
ISLA
DOWN
ANCO
SUMM
VINE
BRIG
6
8
Time : 900 - 1000 LST
Maximum Value = 10.64
Minimum Value = 2.54

Ozone (pphm) 1979 base emissions, July 13, 1979 (pacr1)

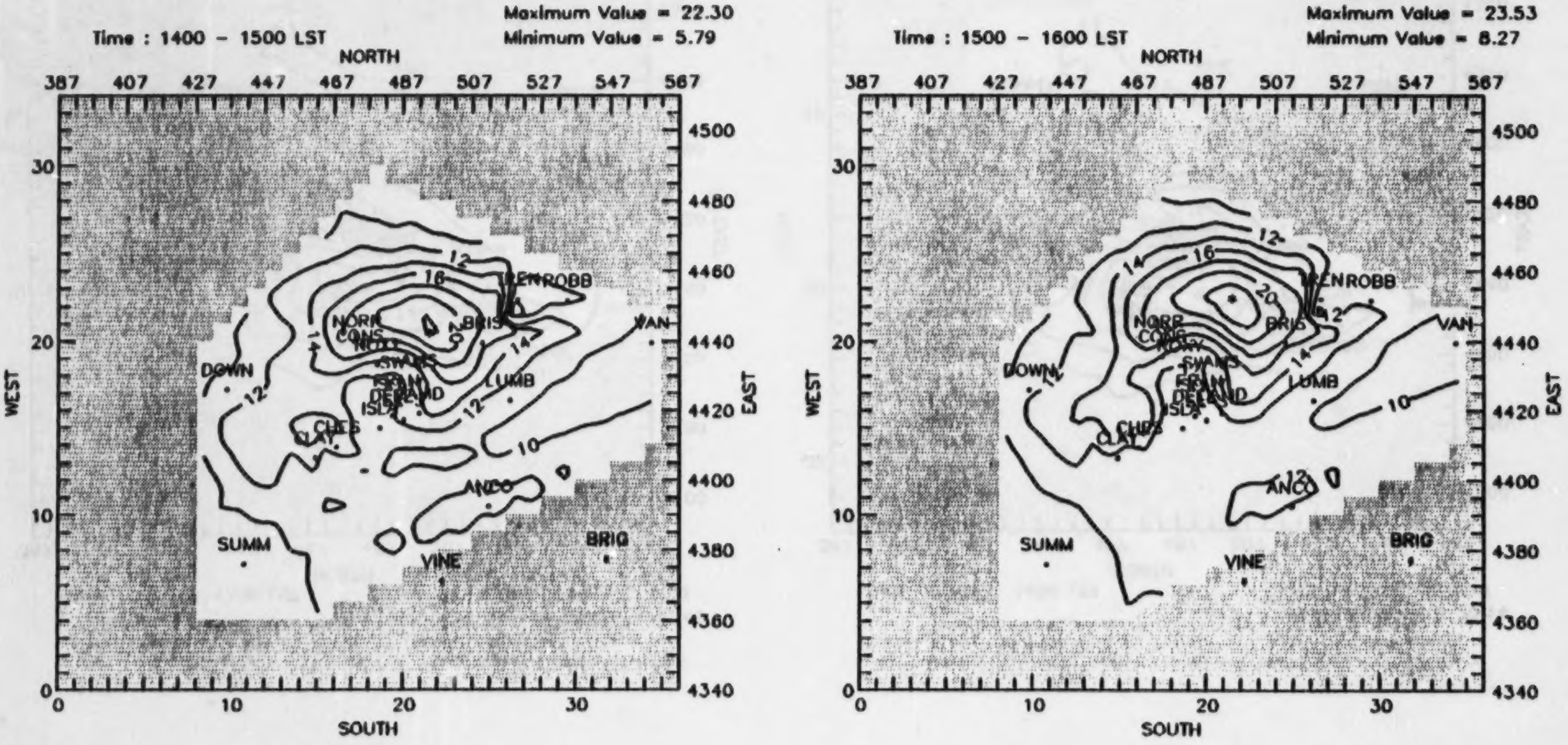


Time : 1000 - 1100 LST
Maximum Value = 12.40
Minimum Value = 2.02
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
0
10
20
30
4340
4360
4380
4400
4420
4440
4460
4480
4500
TRENROBB
NORR
CONS
ROXY
SWAIS
FRAN
DOWN
BRIG
VAN
LUMB
ANCO
VINE
SUMM
10
8
6
Time : 1100 - 1200 LST
Maximum Value = 14.49
Minimum Value = 1.84
12

Ozone (pphm) 1979 base emissions, July 13, 1979 (pacr1)

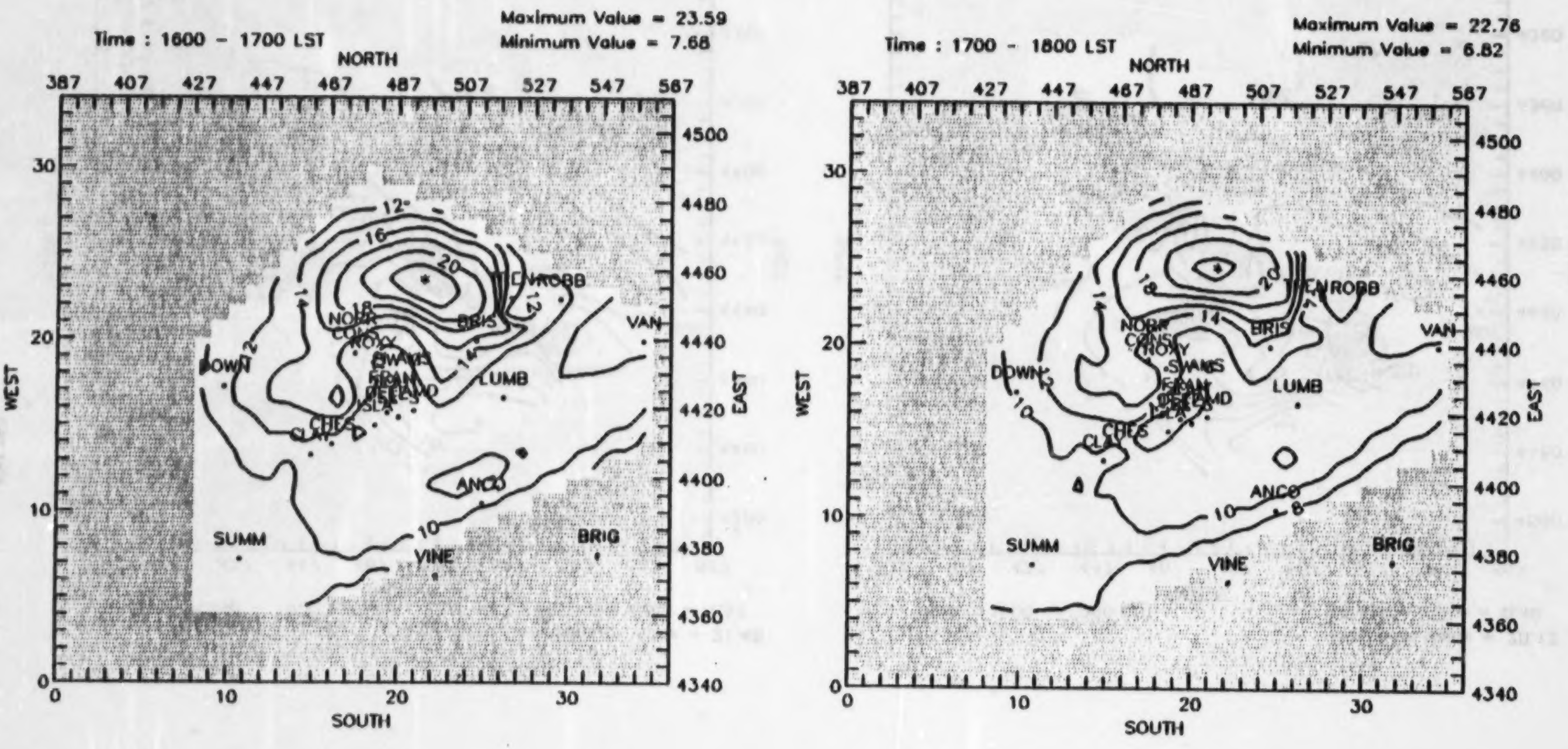

Time : 1200 - 1300 LST
Maximum Value = 17.49
Minimum Value = 1.90
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
DOWN
NORR
CONS
ROXY
SWARS
BRIS
TRENROBB
VAN
LUMB
ISLS
CHES
CLAY
SUMM
ANCO
VINE
BRIG
10
12
14
16
Time : 1300 - 1400 LST
Maximum Value = 20.14
Minimum Value = 4.47

Ozone (pphm) 1979 base emissions, July 13, 1979 (pacr1)

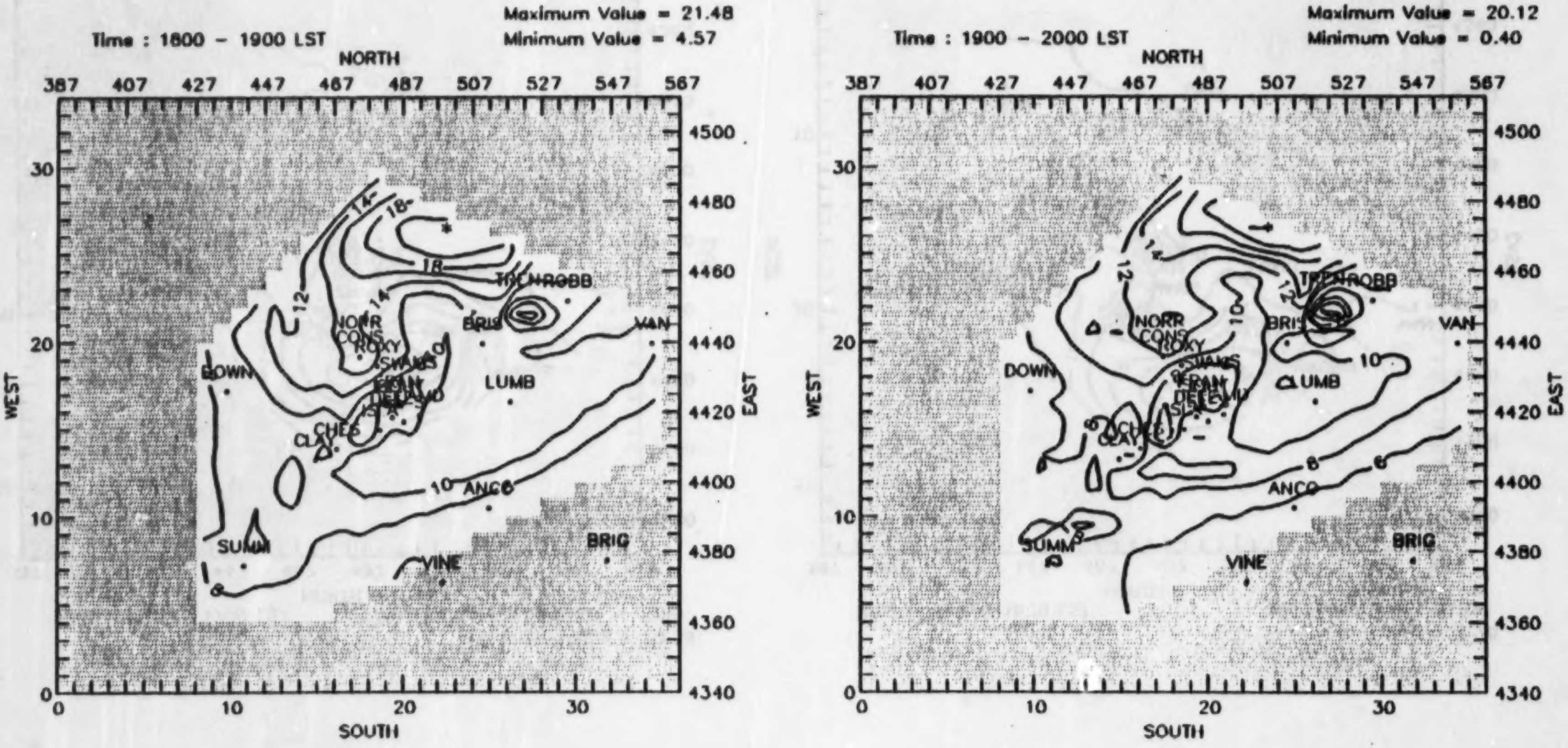


Time : 1400 - 1500 LST
Maximum Value = 22.30
Minimum Value = 5.79
Time : 1500 - 1600 LST
Maximum Value = 23.53
Minimum Value = 8.27
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
DOWN
SUMM
NORR
CONS
NOXY
SWANS
FRAN
DEERPARK
ISL
CHES
CLAY
BRIS
TRENROBB
VAN
LUMB
ANCO
VINE
BRIG
10
12
14
16
20

Ozone (pphm) 1979 base emissions, July 13, 1979 (pacr1)


Time : 1600 - 1700 LST
Maximum Value = 23.59
Minimum Value = 7.68
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
12
14
16
18
20
10
DOWN
NORR
CONS
ROXX
SWANS
FRAN
LUMB
BRIS
VAN
ANCO
SUMM
VINE
BRIG
CHES
CLA
Time : 1700 - 1800 LST
Maximum Value = 22.76
Minimum Value = 6.82
DOWN
NORR
CONS
ROXY
SWANS
FRAN
BRIS
LUMB
VAN
ANCO
SUMM
VINE
BRIG
CHES
CLA
TENROBB
8

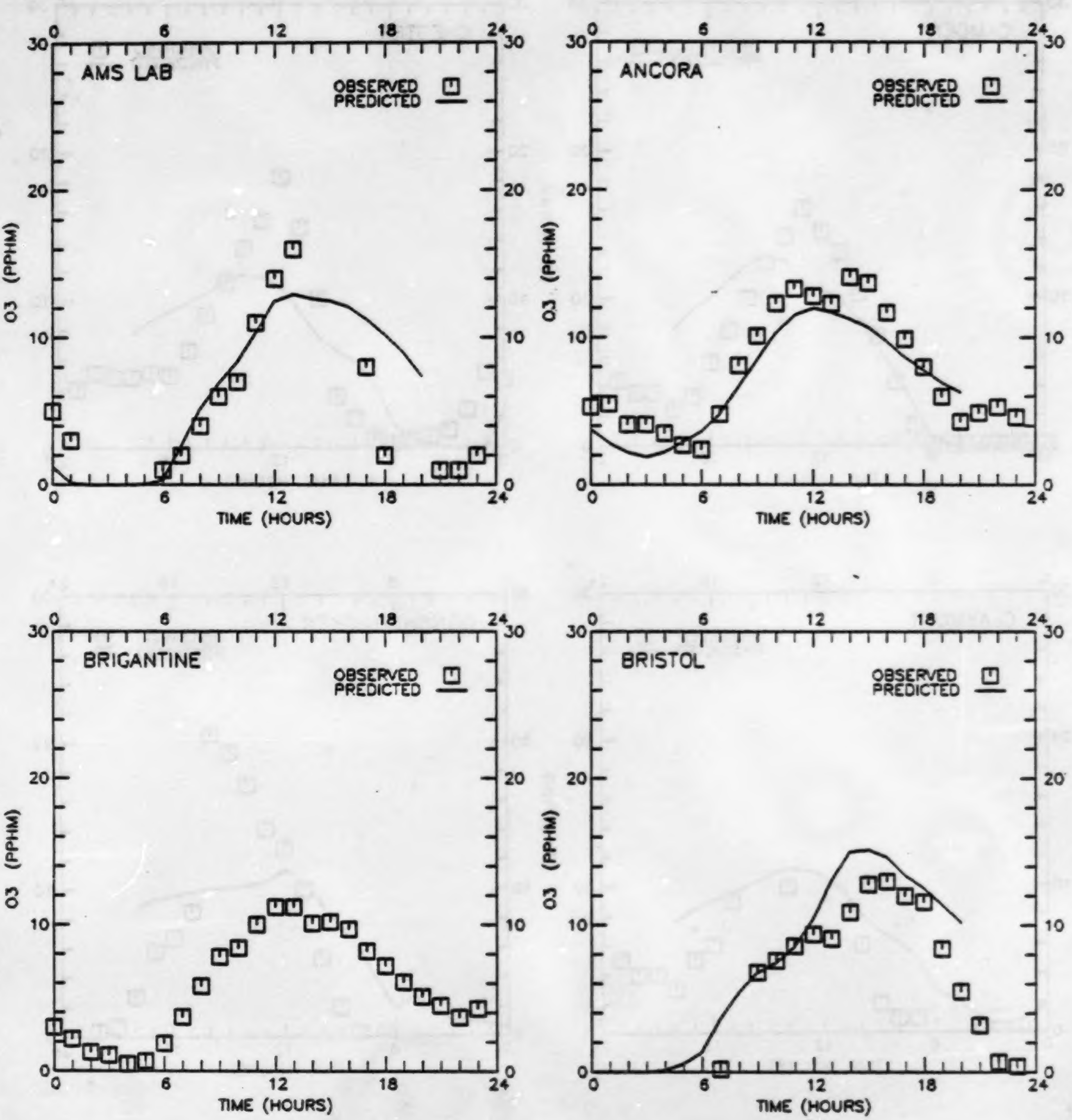
Ozone (pphm) 1979 base emissions, July 13, 1979 (pacr1)


Time : 1800 - 1900 LST
Maximum Value = 21.48
Minimum Value = 4.57
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
0
10
20
30
4500
4480
4460
4440
4420
4400
4380
4360
4340
14
18
18
14
12
10
8
TRENROBB
NORR
CONS
ROXY
SHANS
FRAN
DEFLAUD
BRIS
VAN
DOWN
LUMB
CHES
CLAY
ANCO
SUMM
VINE
BRIG
Time : 1900 - 2000 LST
Maximum Value = 20.12
Minimum Value = 0.40
14
12
10
12
10
8
6
6

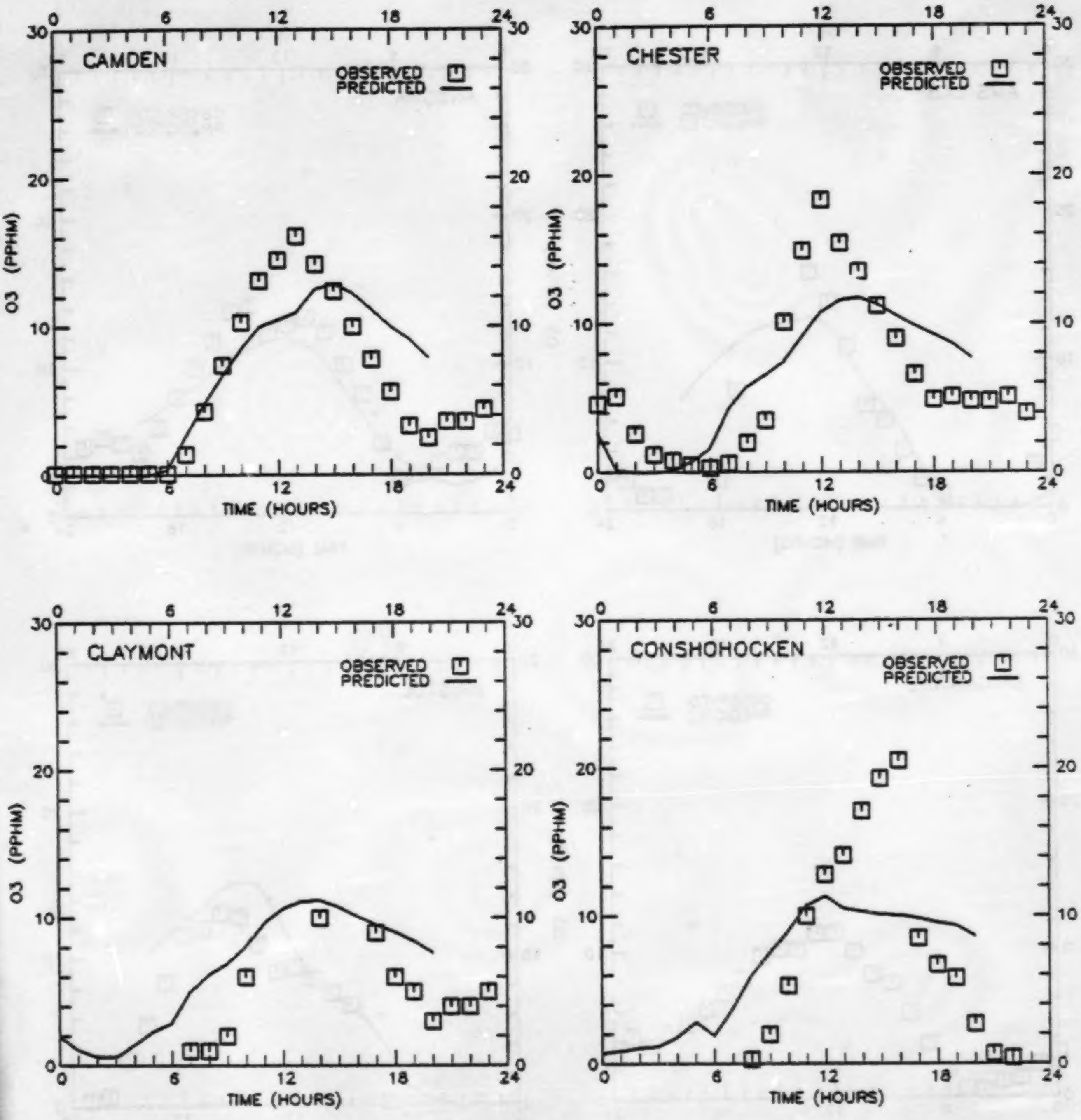
Ozone (pphm) 1979 base emissions, July 13, 1979 (pacr1)

Appendix I

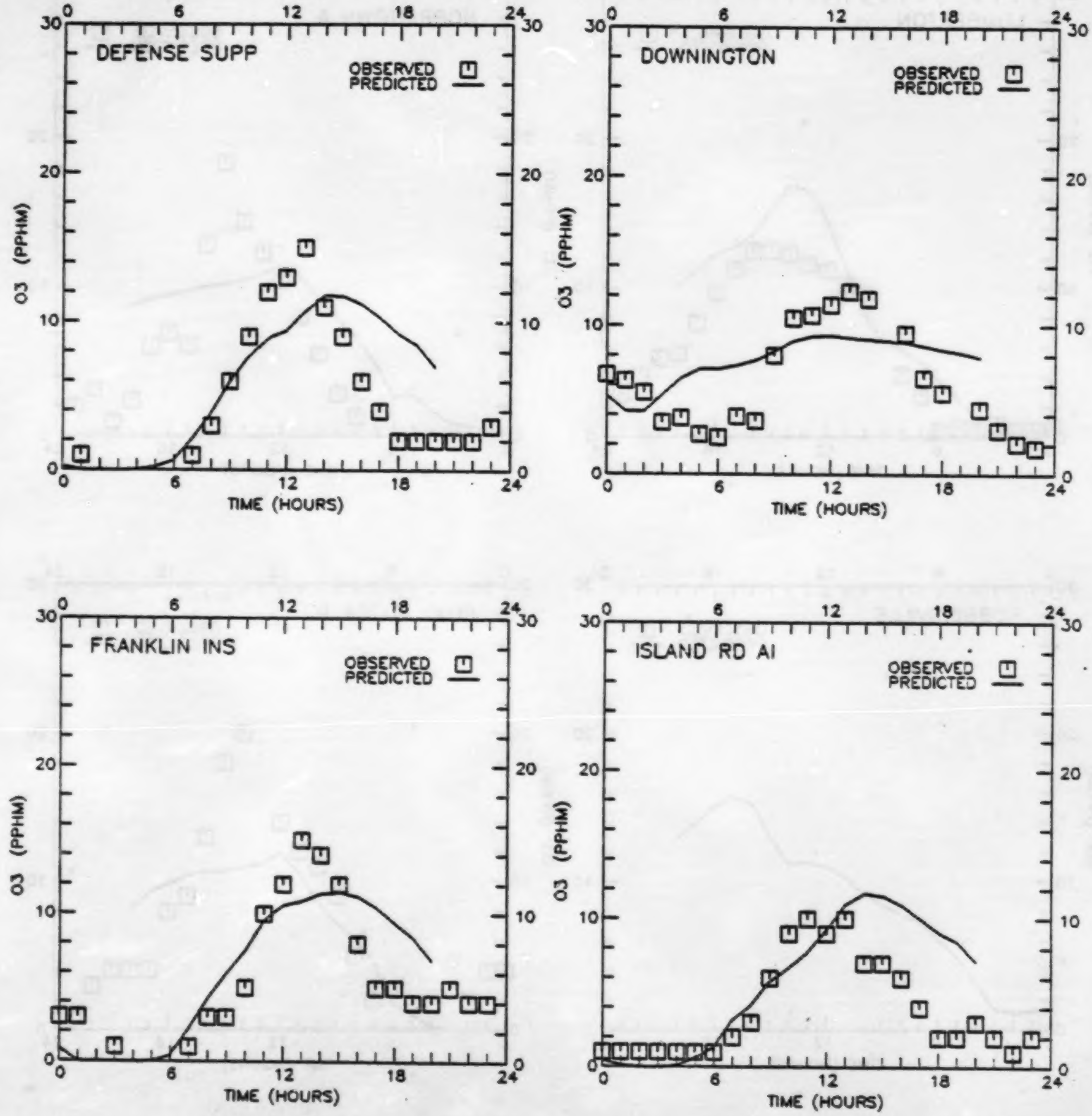
RESULTS OF THE UAM SENSITIVITY TEST FOR PHILADELPHIA USING METEOROLOGICAL INPUTS DEVELOPED FROM A SPARSE DATA BASE (PLANR UAM) AND AIR QUALITY INPUTS DEVELOPED FROM A RICH DATA BASE (POS UAM)



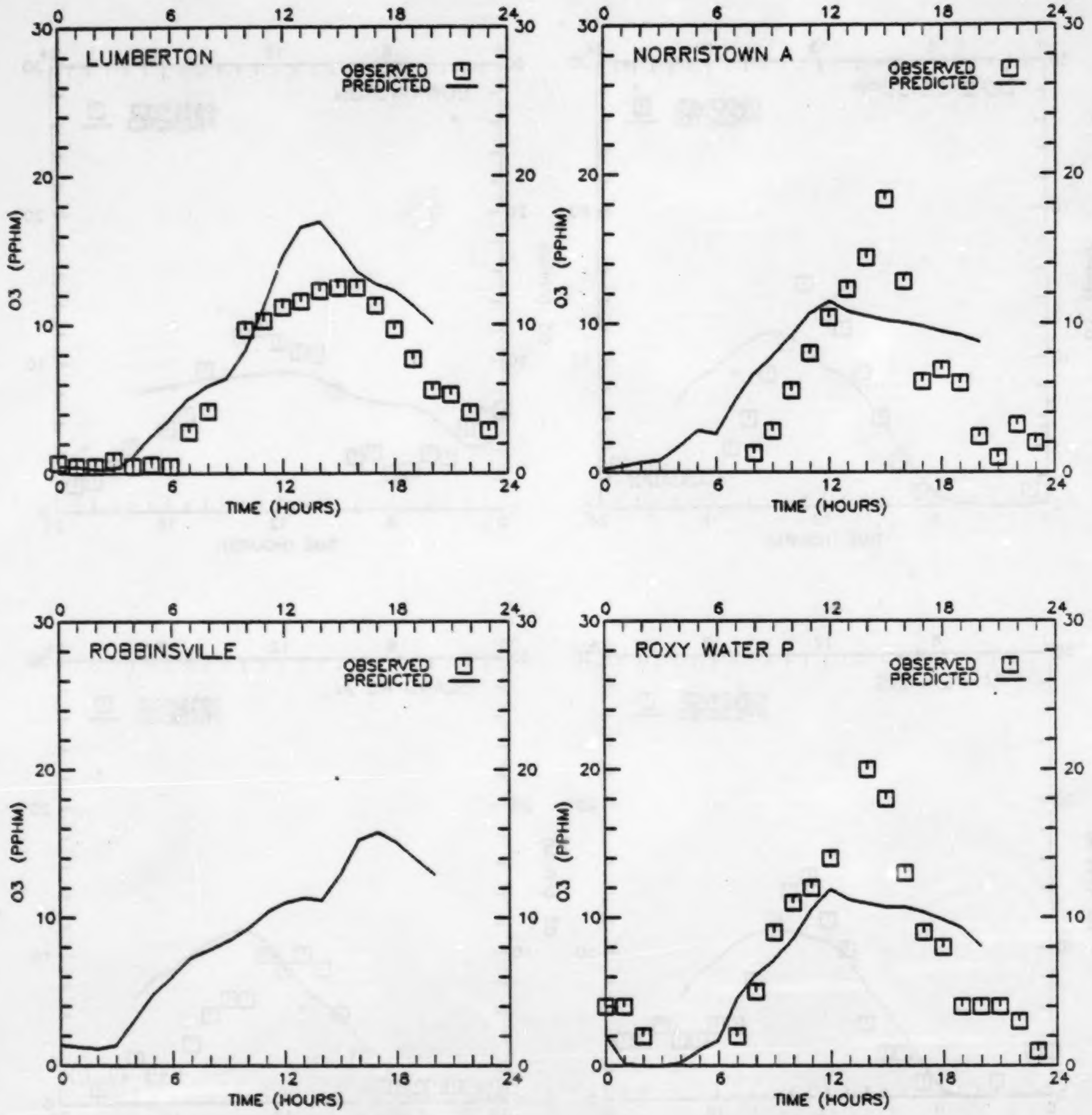
PHILADELPHIA – 7/13/79 – OZ – PLANR RUN #3



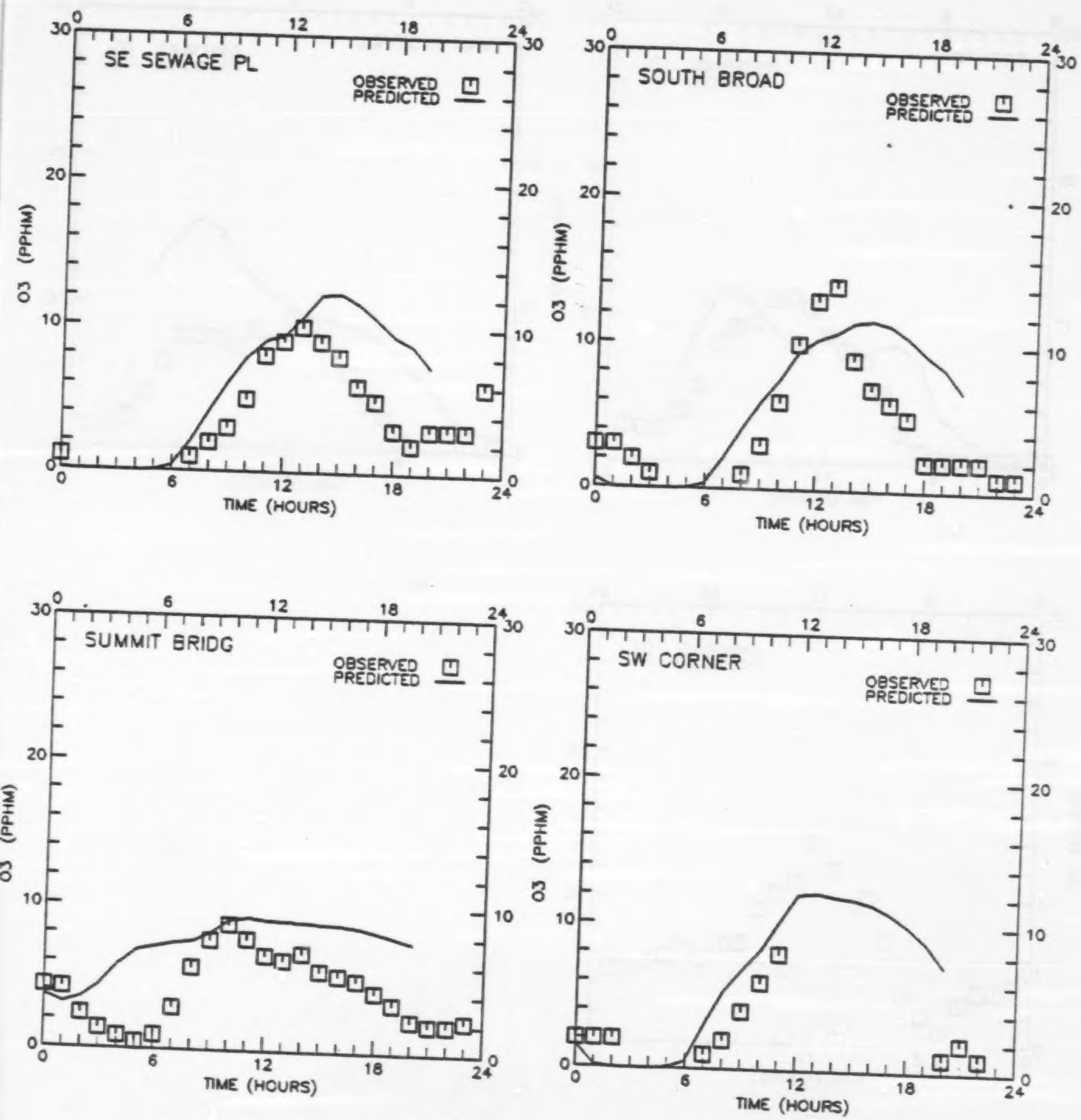
PHILADELPHIA – 7/13/79 – OZ – PLANR RUN #3



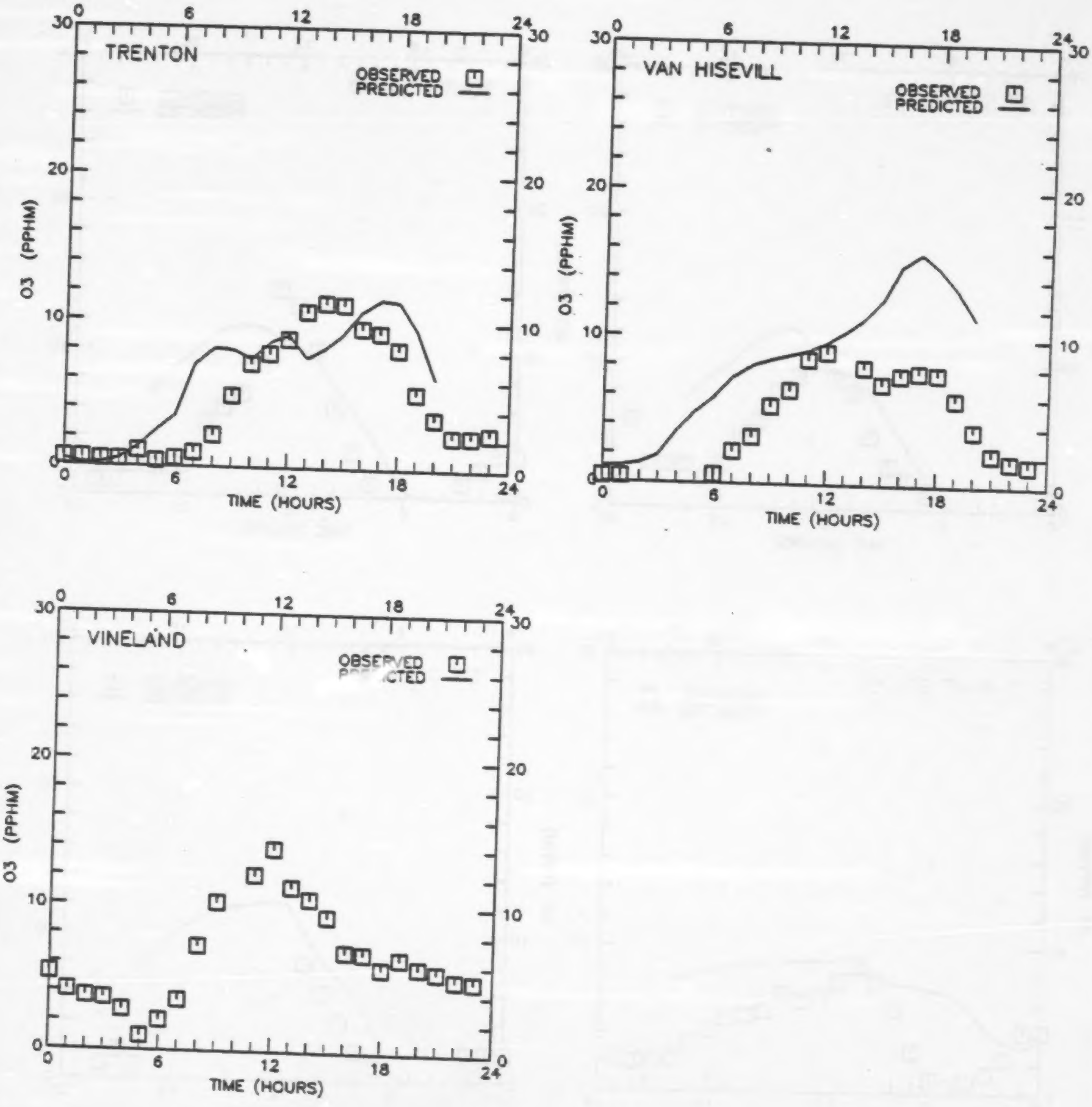
PHILADELPHIA – 7/13/79 – OZ – PLANR RUN #3



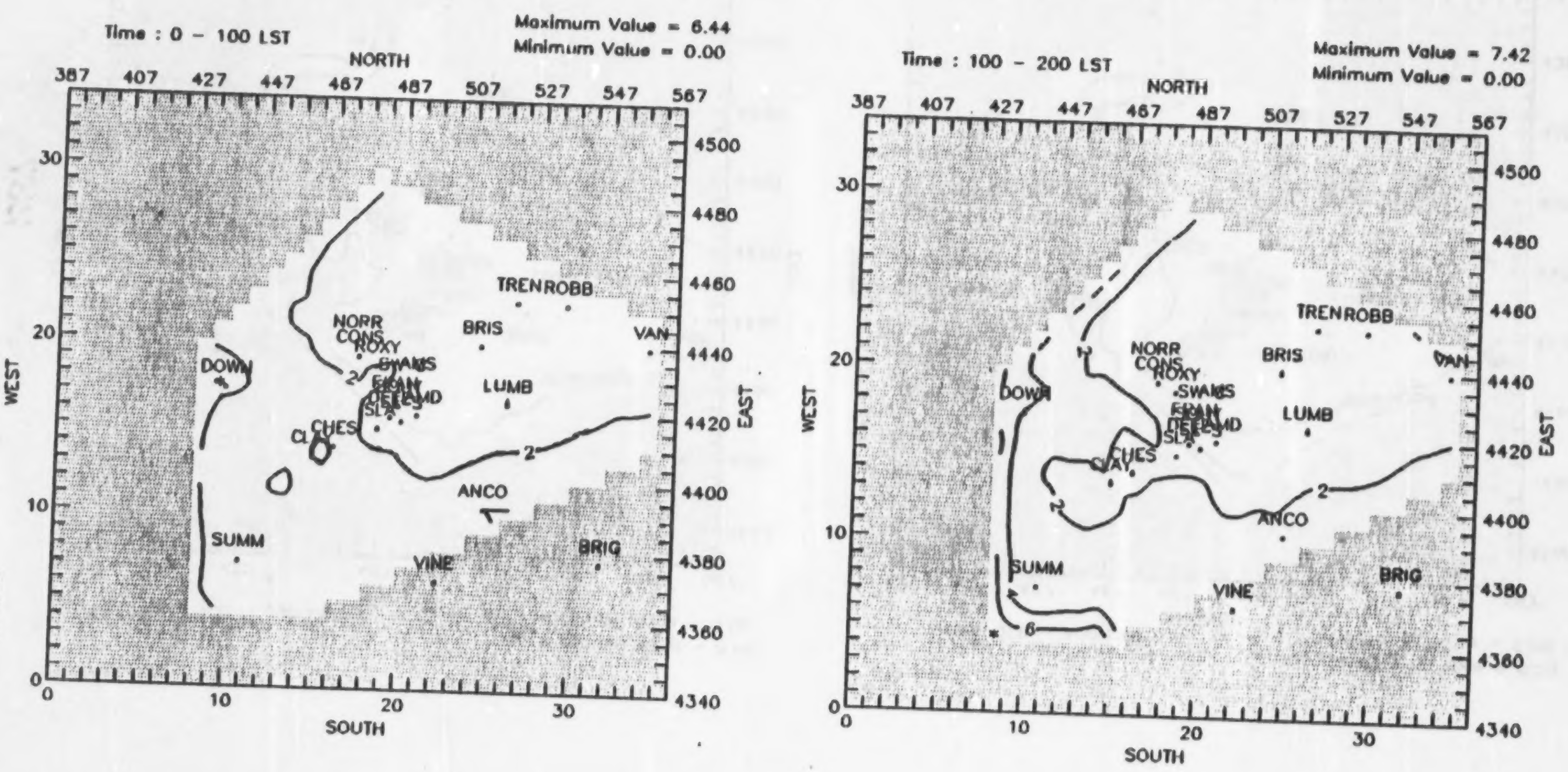
PHILADELPHIA – 7/13/79 – OZ – PLANR RUN #3



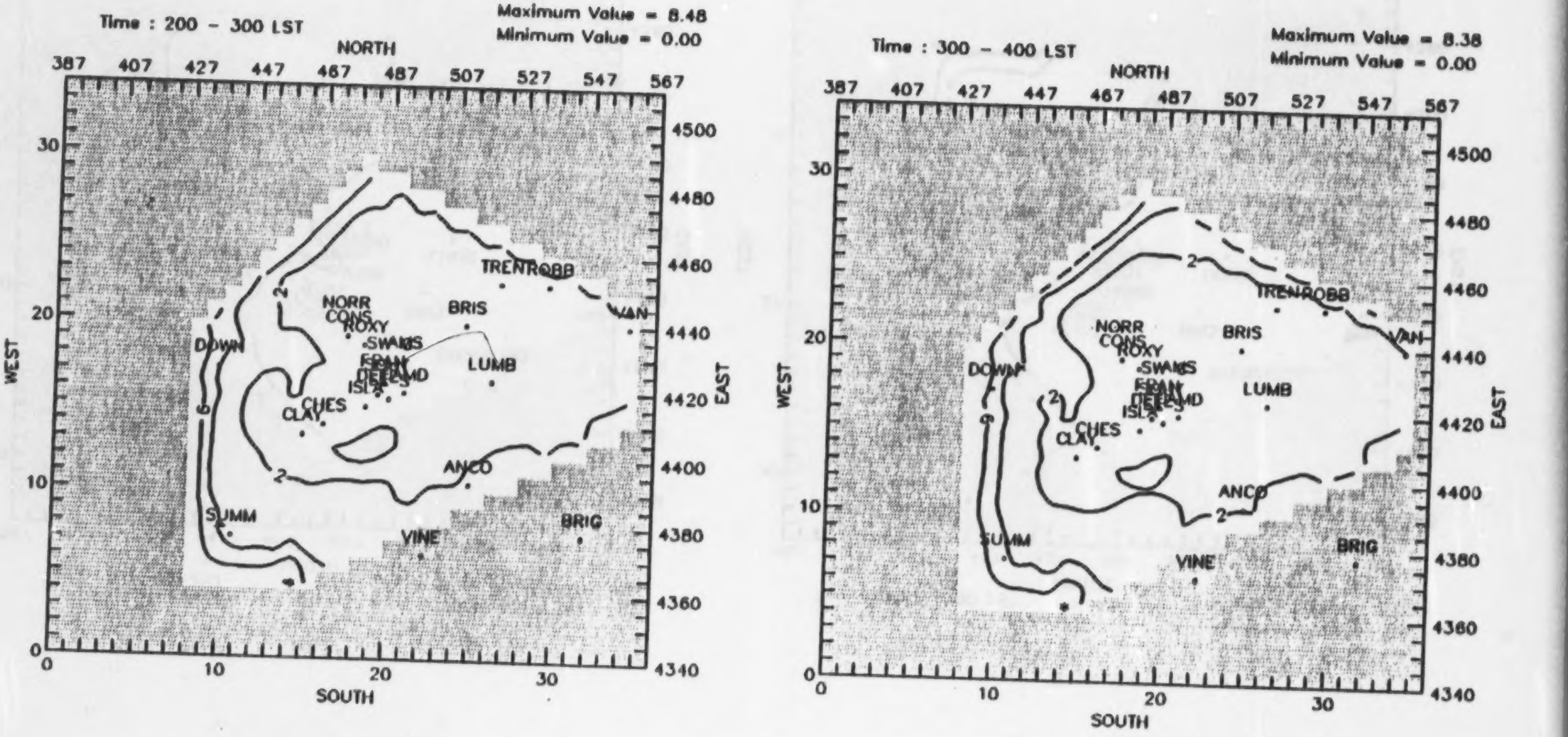
PHILADELPHIA – 7/13/79 – OZ – PLANR RUN #3



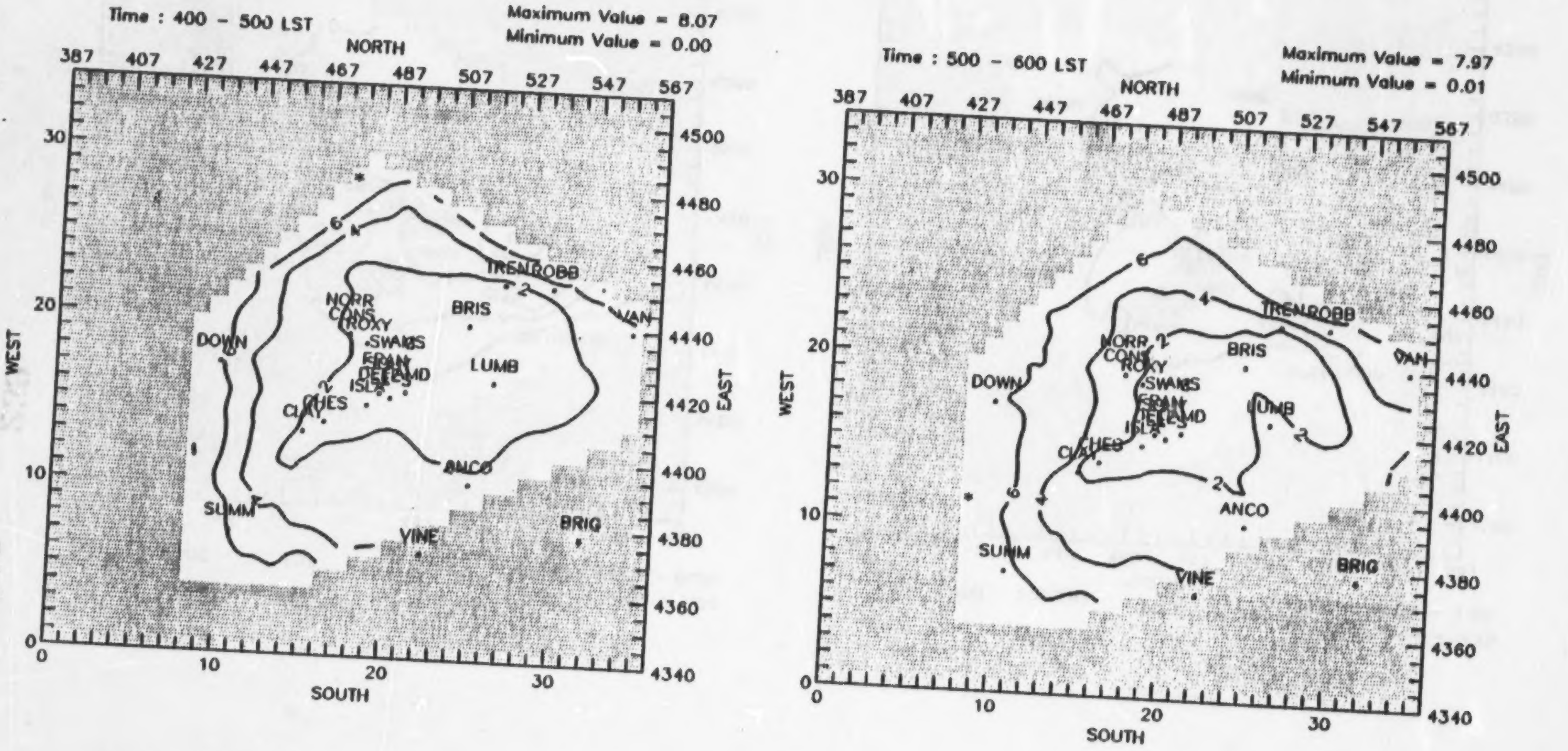
PHILADELPHIA – 7/13/79 – OZ – PLANR RUN #3



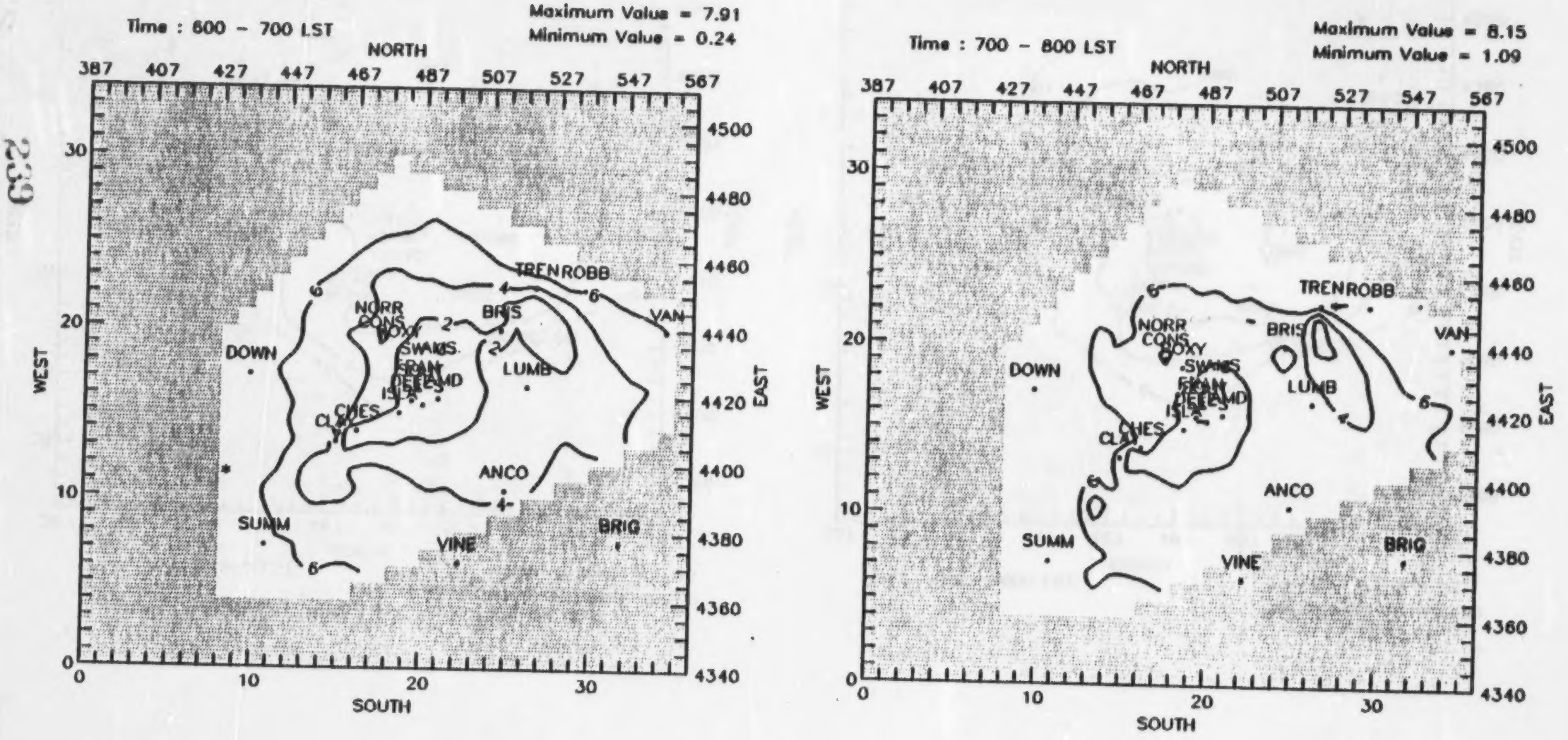
Ozone (pphm), Philadelphia July 13, 1979 (PLANR run#3)


Time : 200 - 300 LST
Maximum Value = 8.48
Minimum Value = 0.00
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
0
10
20
30
4340
4360
4380
4400
4420
4440
4460
4480
4500
TRENROBB
VAN
NORR
CONS
ROXY
SWANS
FRAN
DEEL
CMD
ISLS
BRIS
LUMB
DOWN
CHES
CLAY
ANCO
SUMM
VINE
BRIG
2
6
Time : 300 - 400 LST
Maximum Value = 8.38
Minimum Value = 0.00

Ozone (pphm), Philadelphia July 13, 1979 (PLANR run#3)

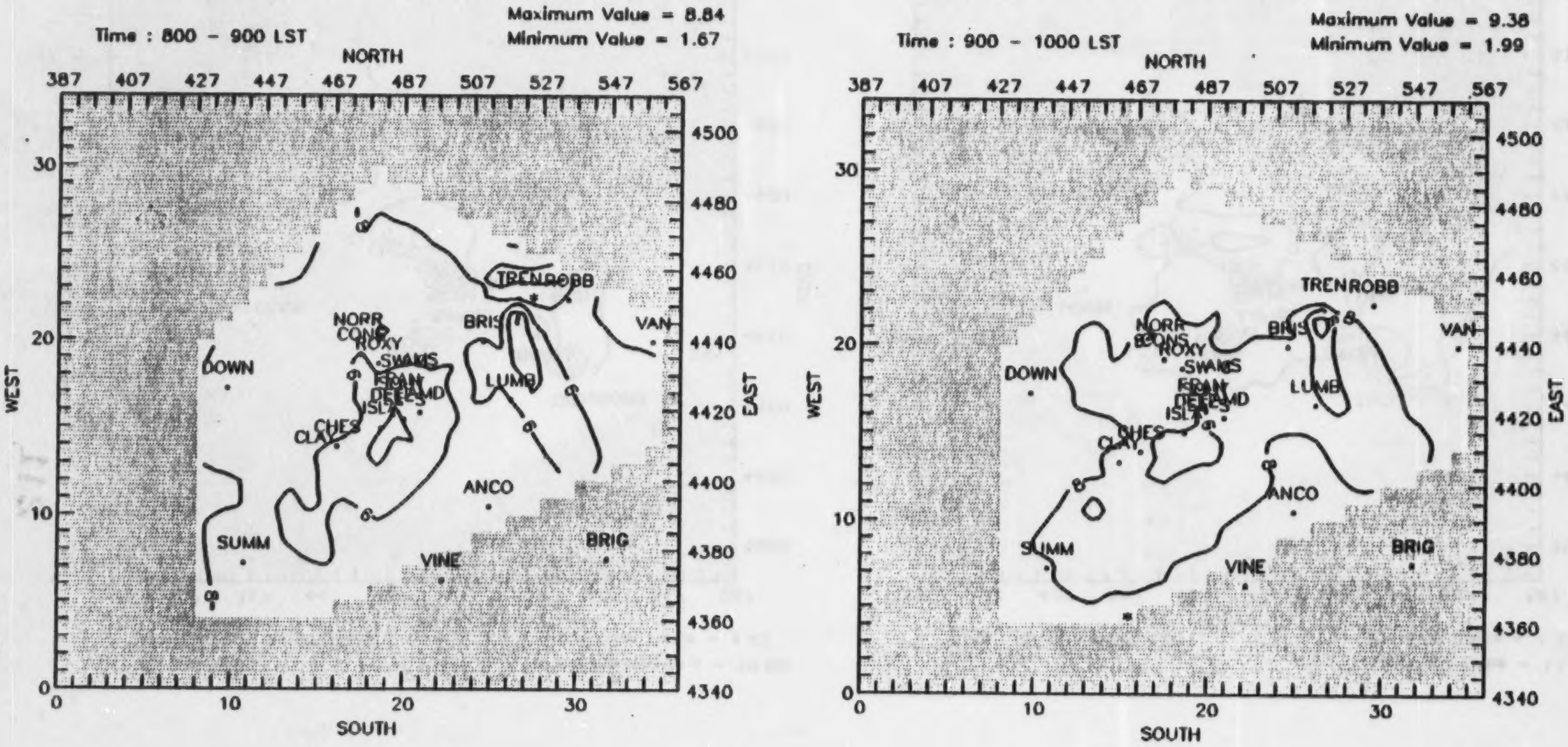

Time : 400 - 500 LST
Maximum Value = 8.07
Minimum Value = 0.00
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
VAN
NORR
CONS
ROXY
BRIS
DOWN
SWANS
FRAN
DELEMD
LUMB
ISLS
CHES
CLAY
ANCO
SUMM
VINE
BRIG
6
4
2
Time : 500 - 600 LST
Maximum Value = 7.97
Minimum Value = 0.01

Ozone (pphm), Philadelphia July 13, 1979 (PLANR run#3)

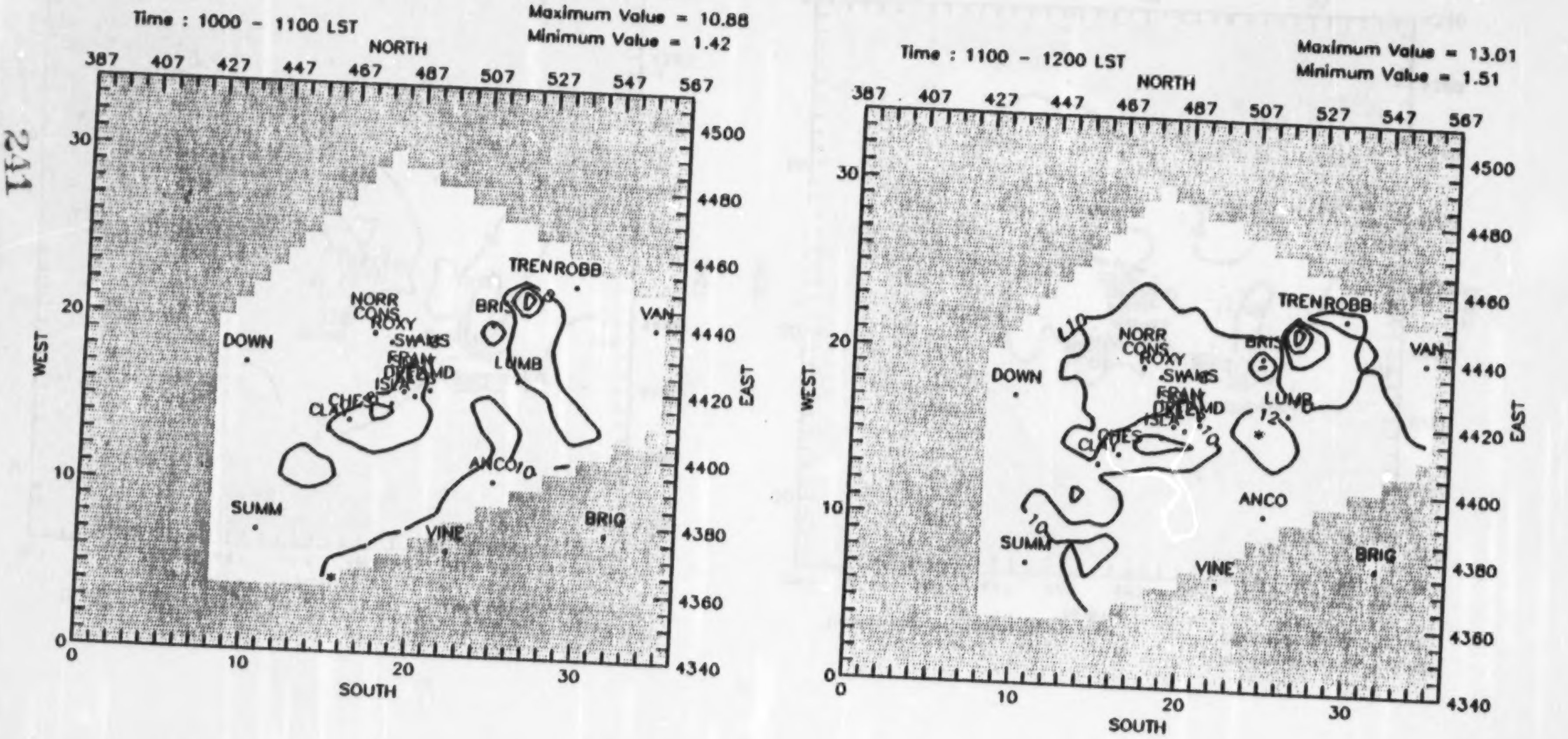


Time : 600 - 700 LST
Maximum Value = 7.91
Minimum Value = 0.24
Time : 700 - 800 LST
Maximum Value = 8.15
Minimum Value = 1.09
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
VAN
BRIS
NORR
CONS
DOXY
SWANS
FRAN
DELEMD
ISLE
CHES
CLAY
DOWN
LUMB
ANCO
SUMM
VINE
BRIG
2
4
6

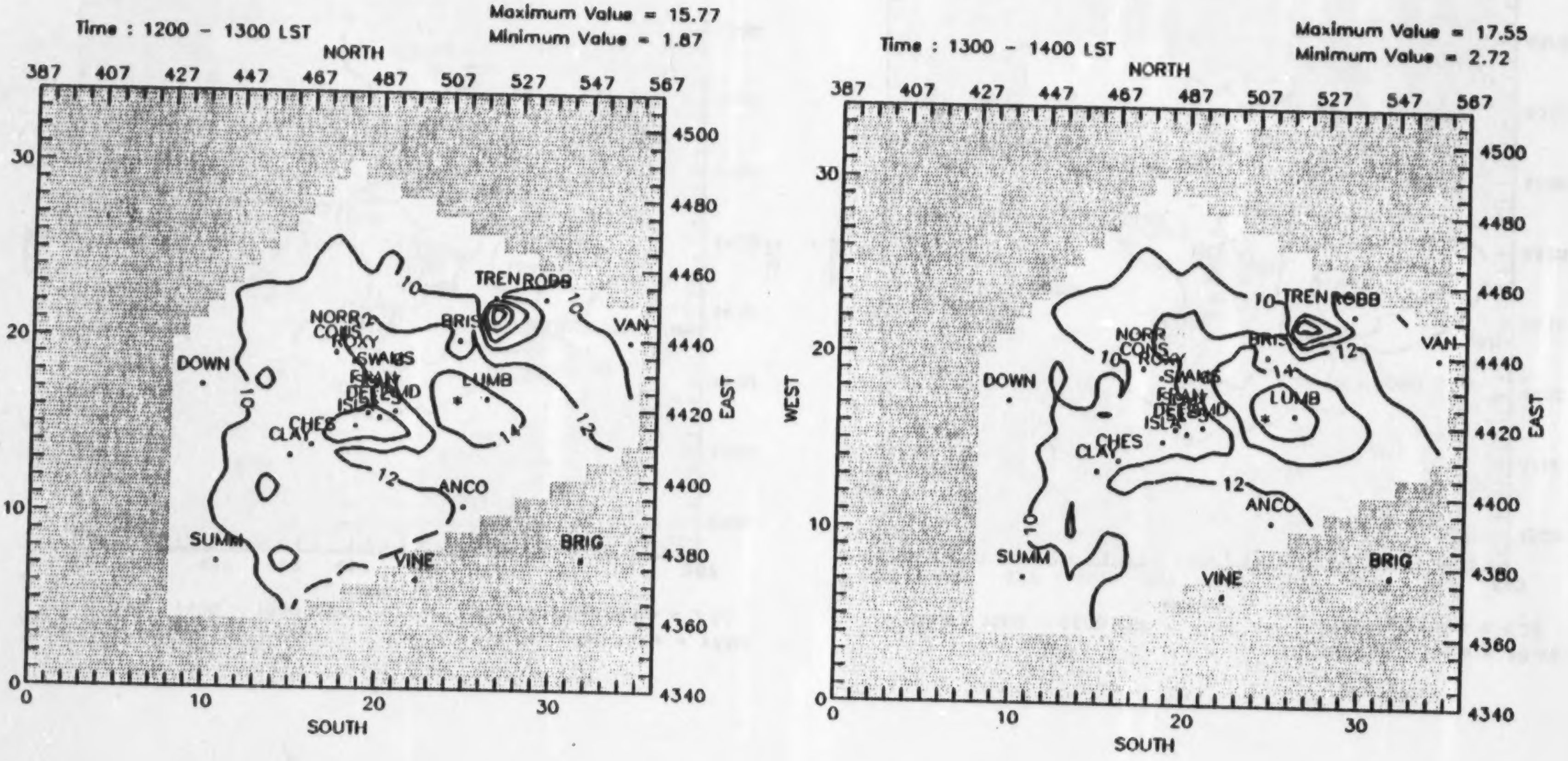
Ozone (pphm), Philadelphia July 13, 1979 (PLANR run#3)


Time : 800 - 900 LST
Maximum Value = 8.84
Minimum Value = 1.67
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
DOWN
SUMM
NORR
CONS
ROXY
SWANS
FRAN
DEFENMD
ISLA
CHES
CLAY
TRENROBB
BRIS
LUMB
VAN
ANCO
VINE
BRIG
Time : 900 - 1000 LST
Maximum Value = 9.38
Minimum Value = 1.99

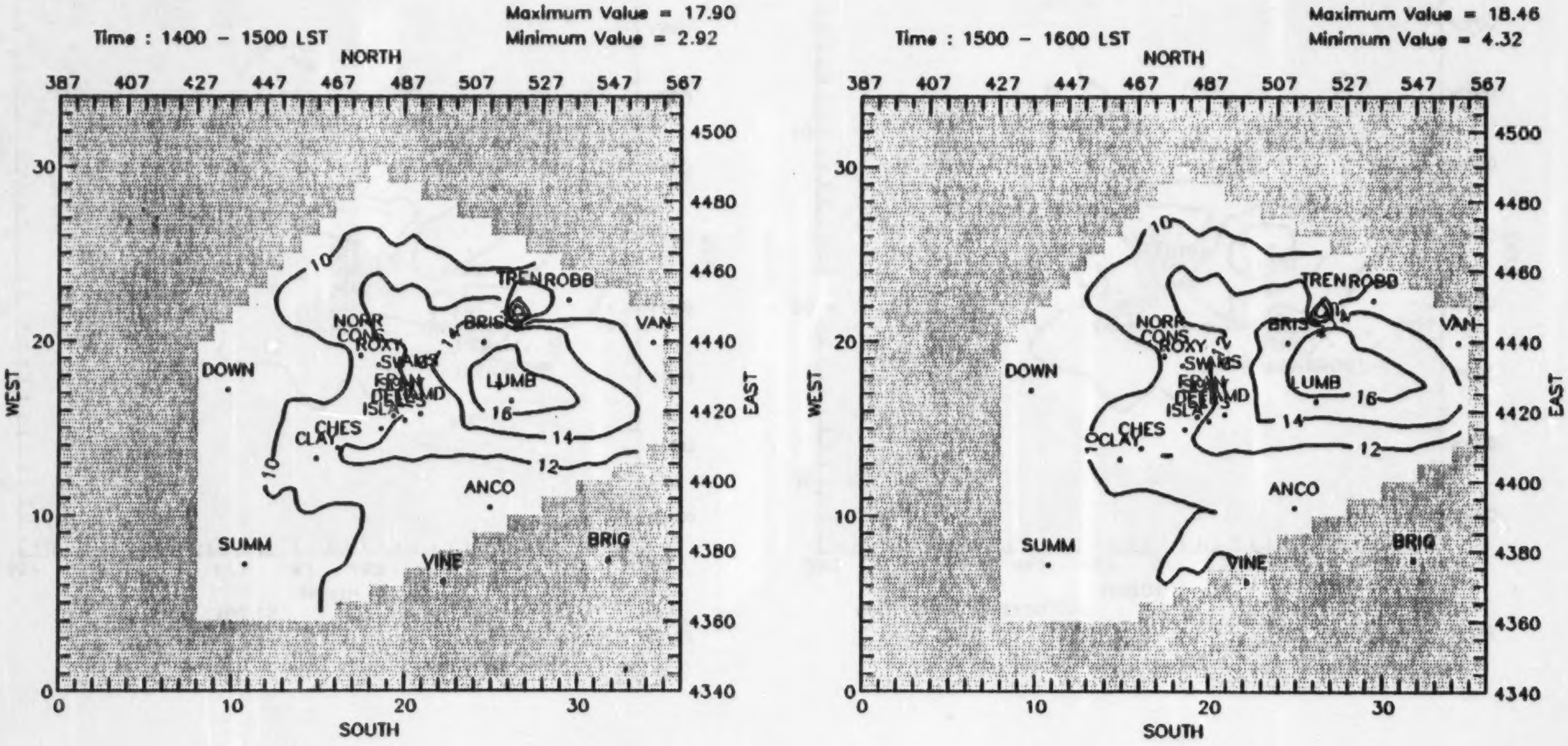
Ozone (pphm), Philadelphia July 13, 1979 (PLANR run#3)


Time : 1000 - 1100 LST
Maximum Value = 10.88
Minimum Value = 1.42
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
DOWN
SUMM
NORR
CONS
ROXY
SWARS
FRAN
DREXMD
ISLA
CHES
CLAY
BRIS
TRENROBB
LUMB
ANCO
VINE
BRIG
VAN
Time : 1100 - 1200 LST
Maximum Value = 13.01
Minimum Value = 1.51
12

Ozone (pphm), Philadelphia July 13, 1979 (PLANR run#3)

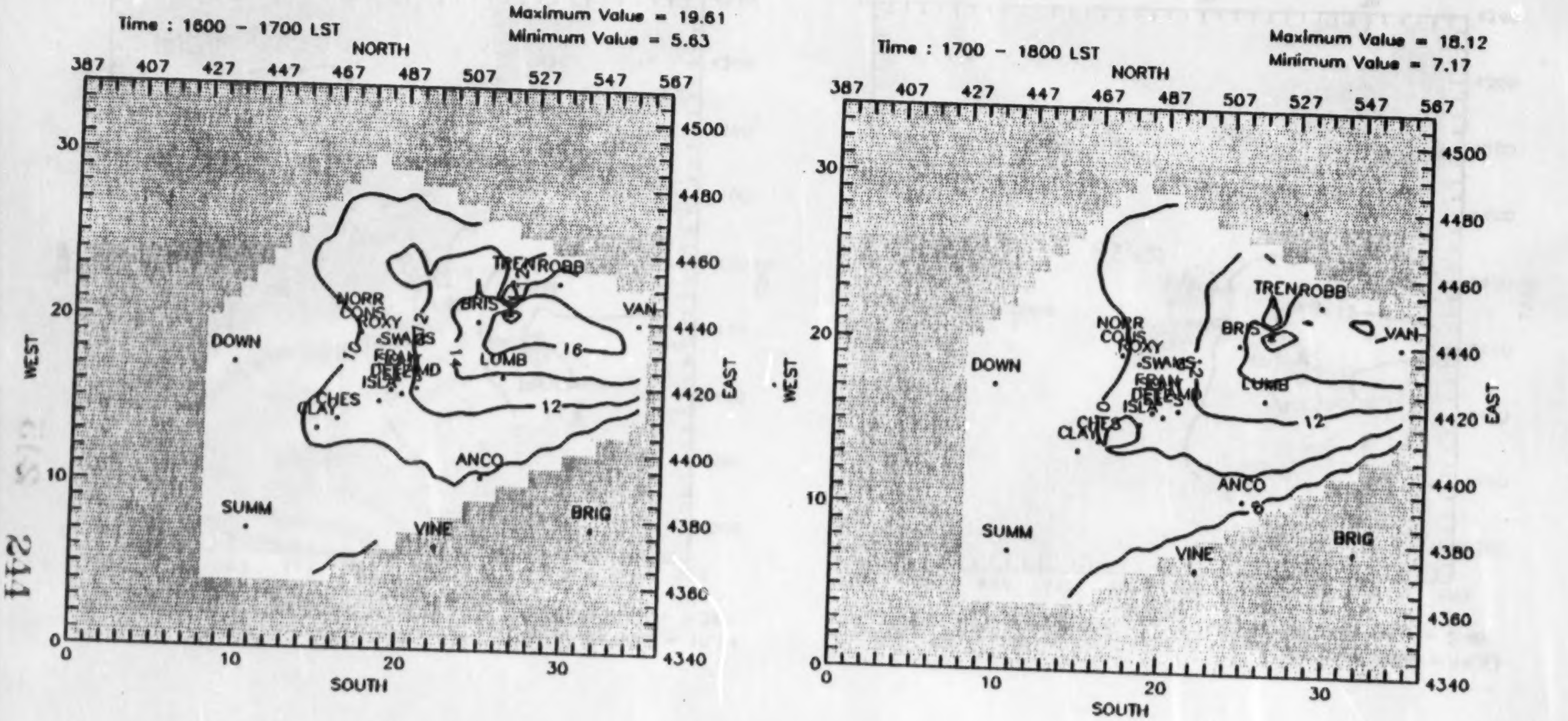

Time : 1200 - 1300 LST
Maximum Value = 15.77
Minimum Value = 1.87
Time : 1300 - 1400 LST
Maximum Value = 17.55
Minimum Value = 2.72
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TREN
ROBB
BRIS
VAN
NORR
CONS
ROXY
SWANS
FRAN
DEFE
LUMB
DOWN
CHES
CLAY
ISLA
ANCO
SUMM
VINE
BRIG
10
12
14

Ozone (pphm), Philadelphia July 13, 1979 (PLANR run#3)

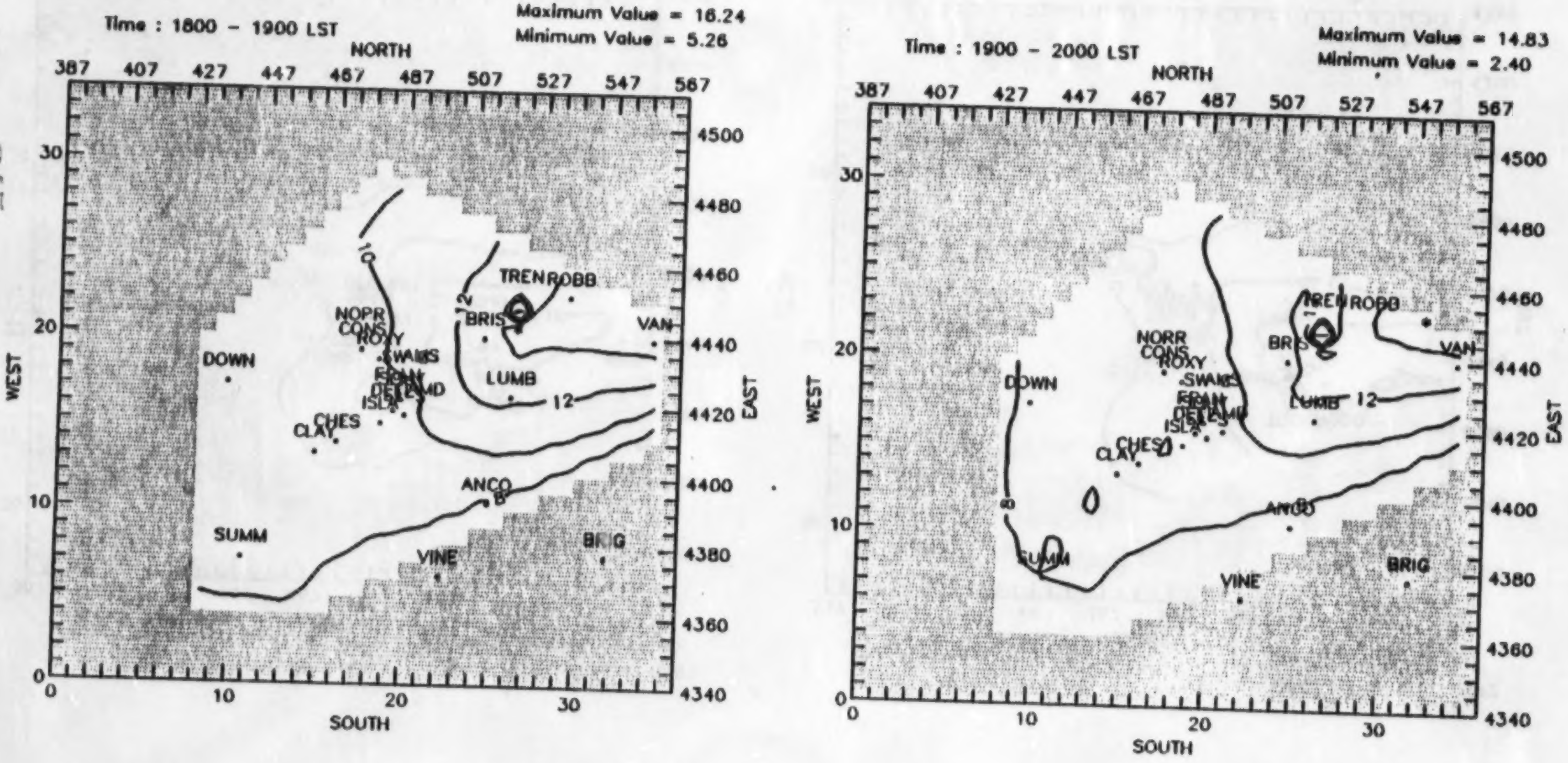


Time : 1400 - 1500 LST
Maximum Value = 17.90
Minimum Value = 2.92
Time : 1500 - 1600 LST
Maximum Value = 18.46
Minimum Value = 4.32
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
BRIS
VAN
NORR
CONS
ROXY
SWANS
FRAN
DELEAMD
ISLA
CHES
CLAY
DOWN
LUMB
ANCO
SUMM
VINE
BRIG
10
12
14
16

Ozone (pphm), Philadelphia July 13, 1979 (PLANR run#3)

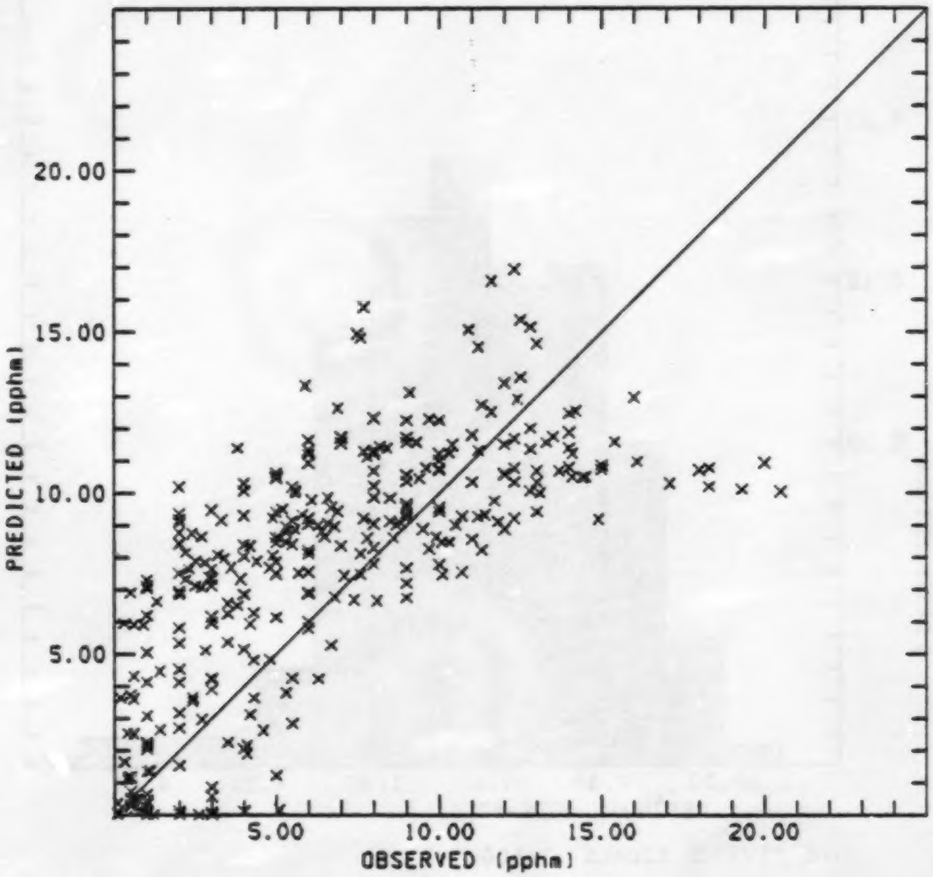

Time : 1600 - 1700 LST
Maximum Value = 19.61
Minimum Value = 5.63
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
0
10
20
30
4340
4360
4380
4400
4420
4440
4460
4480
4500
DOWN
SUMM
NORR
CONS
ROXY
SWANS
FRAN
DEFE
AMD
ISLA
CHES
CLAY
TRENROBB
BRIS
LUMB
VAN
ANCO
VINE
BRIG
10
12
16
Time : 1700 - 1800 LST
Maximum Value = 18.12
Minimum Value = 7.17
NORTH
SOUTH
WEST
EAST
12
8

Ozone (pphm), Philadelphia July 13, 1979 (PLANR run#3)


Time : 1800 - 1900 LST
Maximum Value = 16.24
Minimum Value = 5.26
NORTH
SOUTH
WEST
EAST
387
407
427
447
467
487
507
527
547
567
4500
4480
4460
4440
4420
4400
4380
4360
4340
0
10
20
30
TRENROBB
NOPR
CONS
ROXY
SWAIS
FRAN
DELE
LAMD
ISLA
BRIS
LUMB
VAN
DOWN
CHES
CLAY
ANCO
SUMM
VINE
BRIG
10
12
8
Time : 1900 - 2000 LST
Maximum Value = 14.83
Minimum Value = 2.40
NORR
CONS
ROXY
12
8

Ozone (pphm), Philadelphia July 13, 1979 (PLANR run#3)

VARIABLE...OZONE
BEGINNING DATE...7/13/79
ENDING DATE...7/13/79
OBSERVATION SOURCE...OZONE
OBSERVATION ANALYSIS...AIRS DATA
THE PREDICTION ALGORITHM...PLNR3 UAM(CB-IV) OZONE
AVERAGING TIME...ALL HOURS
STRATITFYING VARIABLE...AIRS DATA SITES
SAMPLE SIZE...330

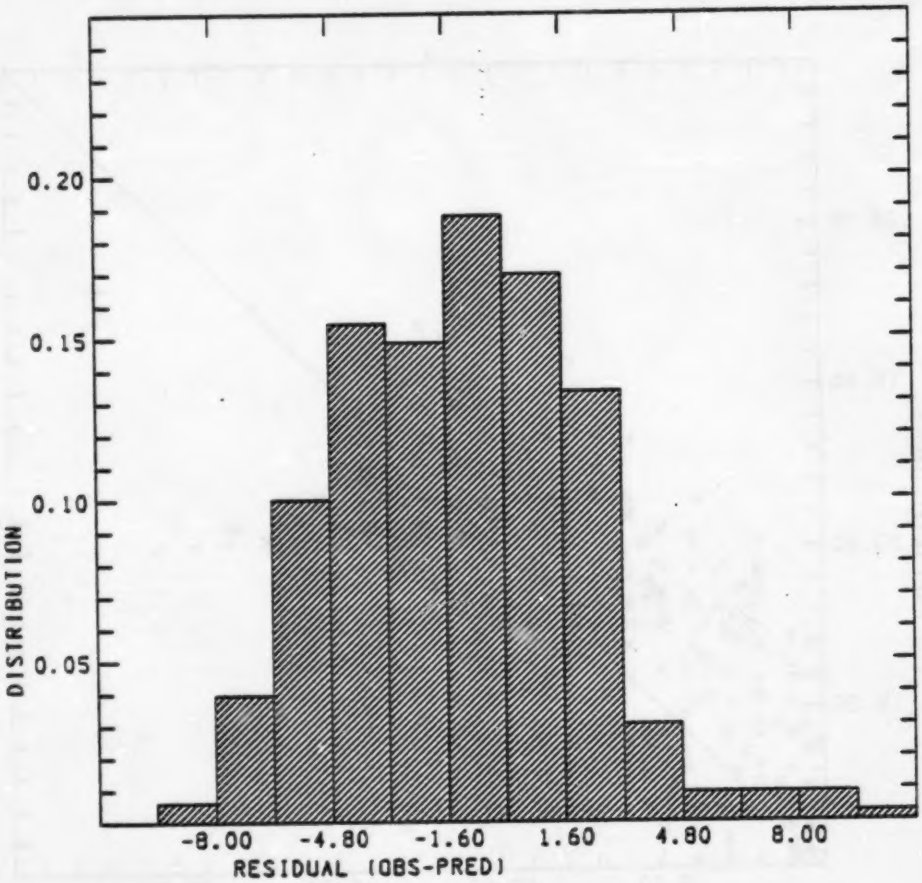


MOMENTS OF THE PROBABILITY DENSITY FUNCTION

	OBSERVED	PREDICTED
AVERAGE	6.22966	7.45774
STANDARD DEVIATION	4.56076	4.02787
SKEWNESS	0.64853	-0.43465
KURTOSIS	-0.28793	-0.62439
OTHER MEASURES		
MEDIAN	5.50000	8.42000
UPPER QUARTILE	9.30000	10.37000
LOWER QUARTILE	2.20000	4.47000
MINIMUM VALUE	0.10000	0.01000
MAXIMUM VALUE	20.50000	16.95000

SKILL OF PREDICTION PARAMETERS
CORRELATION COEFFICIENT OF PREDICTED
VERSUS OBSERVED 0.721
THE BOUNDS OF THE CORRELATION AT THE
CONFIDENCE LEVEL OF 0.050 ARE
LOW BOUND 0.665 HIGH BOUND 0.769
RATIO OF OVER TO UNDER PREDICTIONS 1.750
PERCENT OF OVER PREDICTIONS
GREATER THAN 200 PERCENT OF THE
OBSERVED 22.121
PERCENT OF UNDER PREDICTIONS
LESS THAN 50 PERCENT OF THE
OBSERVED 10.303

```
VARIABLE...OZONE
BEGINNING DATE...7/13/79
ENDING DATE...7/13/79
OBSERVATION SOURCE...OZONE
OBSERVATION ANALYSIS...AIRS DATA
THE PREDICTION ALGORITHM...PLNR3 UAM(CB-IV) OZONE
AVERAGING TIME...ALL HOURS
STRATITFYING VARIABLE...AIRS DATA SITES
SAMPLE SIZE...330
```



THE BINSIZE EQUALS 1.600

```
RESIDUAL ANALYSIS

          AVERAGE           -1.22816
  STANDARD DEVIATION         3.24537
         SKEWNESS            0.37073
         KURTOSIS            0.26506
    OTHER MEASURES
           MEDIAN           -1.18000
      UPPER QUARTILE         0.99000
      LOWER QUARTILE        -3.53000
       MINIMUM VALUE        -8.19000
       MAXIMUM VALUE        10.44000
```

```
BIAS CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND -1.7808
UPPER BOUND -0.6755

STD RESIDUAL CONFIDENCE INTERVAL
AT THE 0.0500 LEVEL
LOWER BOUND 9.3089
UPPER BOUND 12.0307

THE MEASURES OF GROSS ERROR
THE ROOT MEAN SQUARE ERROR IS 3.47
THE AVERAGE ABSOLUTE ERROR IS 2.79

VARIOUS MEASURES OF RELATIVE VARIABILITY
OBSERVATION COEFFICIENT OF VARIATION
                                  0.7321
RESIDUAL COEFFICIENT OF VARIATION
                                  0.5210
RATIO OF RESIDUAL TO OBSERVED ST. DEV.
                                  0.7116
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Appendix J

COMPARISON OF INSTANTANEOUS FAA/NWS WIND VELOCITY OBSERVATIONS WITH HOURLY AVERAGED WIND SPEEDS

Appendix J

COMPARISON OF INSTANTANEOUS FAA/NWS WIND VELOCITY OBSERVATIONS, WITH HOURLY AVERAGED WIND SPEEDS

The UAM requires hourly averaged wind speeds and wind directions, whereas Federal Aviation Administration (FAA) and National Weather Service (NWS) meteorological sites report instantaneous wind observations. When wind varies throughout the hour, the vector averaging of the hourly average wind speeds results in a lower value than the one reported at an FAA/NWS site, which is essentially an instantaneous value taken at the end of an hour. The FAA/NWS wind observations are used primarily to advise pilots of adverse wind conditions at the airport. Thus, during slow wind conditions, which are typical during an ozone episode, the FAA observer may report higher wind gusts that will affect operation. The fact that the hourly average wind speed is calm is of no interest to the pilot if gusts exist that may affect flight operations. This bias of FAA wind speeds was first noticed while developing UAM inputs for the California South Coast Air Basin (SOCAB), where several hourly integrated and FAA wind observation sites are located near each other. A brief analysis of these sites is reported next.

COMPARISON OF HOURLY AVERAGED AND FAA WIND SPEED OBSERVATIONS

During the development of the California South Coast Air Basin (SOCAB) Air Quality Management Plan study four three-day episodes of high ozone days were extensively studied. A systematic bias was seen between the one-hour vector averaged observations at SCAQMD (South Coast Air Quality Management District) surface wind speed monitors and nearby observations of one-minute averaged surface wind speed at FAA/NWS sites. To estimate the extent of the bias, seven NWS/FAA stations were compared with seven SCAQMD wind monitors that were located close to the NWS/FAA stations (i.e., within approximately one UAM grid cell). Table J-1 shows the station pairs and the distance between the FAA/NWS and hourly average stations.

The study periods were the high ozone episodes of 5-7 June, 12-14 August, 21-23 August, and 26-28 August 1985. A total of 1920 collocated data points were collected. This set was reduced by 801 data points because of either a missing station pair or a station pair that was below the speed of 1 knot, the lowest value that FAA/NWS wind monitoring stations can measure.

TABLE J-1. Surface meteorological observation sites and distance between collocated observations pairs.

NWS/FAA Site Name	Location UTM (Zone10)		SCAQMD Site Name	Location UTM (Zone 10)		Distance between Collocated Stations
	UTM_x	UTM_y		UTM_x	UTM_y	
Burbank Airport	356.48	3768.00	Burbank	359.60	3766.40	3.52 km
Los Angeles International Airport	352.48	3744.40	Lennox	354.40	3744.00	1.96 km
Long Beach Airport	370.88	3733.76	Long Beach	368.00	3734.40	2.95 km
El Toro Airport	401.60	3720.16	El Toro	404.8	3716.72	4.70 km
Ontario Airport	411.68	3754.16	Upland	408.00	3758.48	5.67 km
Norton Air Force Base	438.80	3756.96	San Bernardino	434.40	3759.20	4.94 km
Compton Airport	364.40	3740.24	Lynwood	366.40	3743.20	3.57 km

The mean value for the remaining 1119 data points for the FAA/NWS stations was 3.49 m/s, while the mean for the SCAQMD stations was 1.93 m/s, suggesting that the FAA/NWS stations were biased by approximately 45 percent (i.e., the hourly average wind speeds were a little over half of the FAA instantaneous observations). The differences in the median values were also very similar, with values of 3.10 m/s for FAA/NWS stations and 1.80 m/s for SCAQMD stations. Each day was examined to see if any particular day showed an extreme bias; the bias ranged from 36 percent on 13 August to 51 percent on 26 August.

Similarly, all seven stations were examined to see if any particular station may have been the cause of the bias. Five of the seven stations showed a similar bias, ranging from 45 to 56 percent. However, two pairs showed a significantly smaller bias; the Upland site and Ontario Airport pairs showed a bias of only 28.8 percent, and the San Bernadino site and Norton Air Force Base pair showed a bias of only 2.4 percent. In an attempt to see if the agreement was caused by low nighttime wind speeds at Norton Air Force Base, the wind observations during the daytime period were analyzed and almost no bias occurred for the San Bernadino-Norton Air Force pair. The possibility exists that the data may have been incorrectly processed or reported; for example, incorrect conversion from knots to m/s could account for the small bias.

We believe that the one-minute average wind speeds reported from FAA/NWS stations are correct. As a result of the SCAQMD study, which may be true for other locations also, it was concluded that FAA/NWS surface wind observations may have a positive bias of as much as a factor of 2.

This preliminary analysis is by no means complete or statistically roboust. However, it does have important implications for the development of wind fields for air quality simulations models, such as the UAM. It also helps explain some of the UAM's tendency to underpredict peak ozone concentrations at some locations in the past, e.g., St. Louis and Philadelphia. Further analysis of the SCAQMD wind data base and data from other locations is necessary to determine the extent and frequency of this bias. For example, hourly average wind speeds are calculated by vector averaging of a series of lower frequency wind observations. A comparison of one-minute wind speeds with the hourly average wind speed may give some indication of the extent of the bias.